# Multi-scale modeling of liquid transport in fibrous materials

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**Abstract**

Ising's model, combined with Kawasaki dynamics, is applied in modeling liquid transport in fibrous materials. To bridge the gap between the macro behavior of a heterogeneous material system and its basic constituent particles, an attempt at the multi-scale modeling of transport in fibrous materials is presented in this paper.

*Keywords:* Multi-scale modeling; Fibrous materials; Ising's model; Kawasaki dynamics

## 1. Introduction

An old topic with its latest applications in such critical areas as nano-fibrous materials for absorption, bio-filtration/purification, and liquid transport in fibrous materials has been attracting much research interest. Up to now, most efforts in this field have been based on macroscopic phenomena and have used empirical methods [1,2,3,4,5]. Since the 1990s, non-homogeneous flows have also been studied using stochastic simulation [6]. This simulation is based on the so-called Ising's model and Kawasaki dynamics. Recently it has been used in the simulation of wetting dynamics in heterogeneous fibrous structures [7,8,9,10].

In this paper, Ising's model combined with Kawasaki dynamics is further developed to bridge the gap between the macro behavior of a heterogeneous material system and its basic constituent particles, resulting in an attempt at multi-scale modeling. This will provide a useful tool in studying material systems with a characteristic length scale in the range of micros and nanos.

## 2. Model description

### 2.1. Ising's model

In statistical thermodynamics, the macro characteristics of a system are a reflection of the interactions and resulting balance among micro particles/cells that comprise the system. In Ising's model, a system is divided into a number of lattice cells. Then the Hamiltonian is calculated as the summation of the interactions between each pair of closest neighboring cells. The macroscopic parameters of the system can be derived from the Hamiltonian via statistical mechanics. The advantage of Ising's model is that, by its simple expression, it can be used to describe a complex system made of subsystems with two interchangeable configurations.

In a two-dimensional Ising's model for liquid transport, the field is divided into a lattice of $L \times L$ square cells. Two variables are used to describe the state of each cell in the lattice:

(i) $s$ is used to describe whether a cell is occupied by liquid (denoted by 1 if occupied, otherwise 0).
(ii) $F$ is used to describe whether a cell is occupied by the fibrous media (1 if occupied, otherwise 0).

The total Hamiltonian of the system, $H$, is considered as a sum of all the contributions of the cell energies $H_i$ in the lattice:

$$H_i = -\left(B_0 \sum_i s_i F_i + B_1 \sum_{i,j} s_i F_j\right) - C \sum_{i,j} s_i s_j + G \sum_i s_i y \tag{1}$$

where the terms in the bracket represents the interaction between liquid/fiber cells, and the coefficients $B_0$ and $B_1$ are the adhesive energy between fiber/liquid. The second

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term represents the interaction between liquid cells, and $C$ is the liquid cohesive energy. The last term represents the effect of gravity, of which $G$ is the intensity of the gravity and $y$ the $y$-coordinate of the cell in the lattice.

### 2.2. Kawasaki dynamics

The evolution of the system is directed by minimization of the system Hamiltonian, $H$, expressed in Eq. (1). The minimization of $H$ is based on descent steps caused by spin exchanges that obey Kawasaki dynamics [11]. Consider a thermodynamics system connected to a thermodynamics reservoir, and energy exchange can occur between them. This canonical ensemble is governed by the Boltzmann distribution of the state probability ratio [7,11]:

$$\frac{P(H_a)}{P(H_b)} = \Lambda = \exp\left(-\frac{H_b - H_a}{\tau}\right) \tag{2}$$

where $\tau$ is proportional to the absolute temperature, $P(H_k)$, ($k = a$ and $b$) is the probability that the system exists in a configuration with energy $H_k$. $\Lambda$ is a measure of the probability for the system to change its configuration, through spin exchange from a state with energy $H_a$ to a state with $H_b$.

In Kawasaki dynamics, two randomly chosen spins $s_i$ and $s_j$ of different values $+1$ and 0 are considered. The system Hamiltonians are calculated for cases before ($H_a$) and after ($H_b$) the spin exchange. A random number $r$ is then chosen from the interval (0, 1). In the case $r$ is less than the energy barrier ($r < \Lambda$), these two spins will exchange their position. This simulation method involving the generation of random numbers is also known as the Monte-Carlo method.

## 3. Multi-scale modeling of liquid transport in fibrous materials

A 'meso-scale' approach, Ising's model bridges the gap between the behavior of a material at the macro scale and the interactions of its constituent micro-components. In other words, the macro behavior of a material can be predicted from the micro-interactions of its basic particles by a hierarchy of modeling approach with descending scales, also known as multi-scale modeling.

This multi-scale modeling is especially useful in the study of materials with a characteristic length scale in nanos/micros, as it is reported that there are limitations to the conventional continuum mechanics approach (e.g. the FEM) to describe the behavior of materials at scales of micros [12]. Currently, the transition from one scale to another in a multi-scale approach is usually carried out by a 'hand-shaking strategy' [12,13], that is, the information gained from a lower scale is summed into a finite set of parameters, and passed onto the higher scale.

In the following section, an attempt at the multi-scale modeling of transport in fibrous materials is presented, going through from quantum field theory, to statistical mechanics, and then to continuum methods.

### 3.1. From quantum field theory to statistical mechanics

The coefficients $B_0$, $B_1$ and $C$ in Eq. (1), which are essential for the input to Ising's model for transport, are determined in a manner as described as follows.

First, we assume that the van der Waals forces dominate the interactions between fiber and liquid. According to the Lifshitz theory [14], the interaction energy per unit area between two surfaces is

$$W_{1,2} = -h_{1,2}/12\pi D^2 \tag{3}$$

where $h_{1,2}$ is the Hamaker constant, and $D$ the distance between the surfaces. Derived from the quantum field theory, an approximate expression for the Hamaker constant of two bodies (1 and 2) interacting across a medium 3 is

$$h_{1,2} = \frac{3\mathrm{h}\nu_e\left(n_1^2 - n_3^2\right)\left(n_2^2 - n_3^2\right)}{8\sqrt{2}\left(n_1^2 + n_3^2\right)^{1/2}\left(n_2^2 + n_3^2\right)^{1/2}\left\{\left(n_1^2 + n_3^2\right)^{1/2} + \left(n_2^2 + n_3^2\right)^{1/2}\right\}} + \frac{3}{4}\mathrm{k_B}T\frac{\varepsilon_1 - \varepsilon_3}{\varepsilon_1 + \varepsilon_3}\cdot\frac{\varepsilon_2 - \varepsilon_3}{\varepsilon_2 + \varepsilon_3} \tag{4}$$

where $n_i$ is the refractive index of phase $i$, and $\varepsilon_i$ is the static dielectric constant of phase $i$. Constants $k_1$ and $k_2$ are used to represent the ratios of $B_1/C$ and $B_0/B_1$, respectively:

$$k_1 = \frac{B_1}{C} = \frac{W_{1,2}}{W_{1,1}} = \frac{h_{1,2}}{h_{1,1}}, \quad k_2 = \frac{B_0}{B_1} = \frac{W_{1,2}\pi dal}{W_{1,2}a^2} = \frac{\pi dl}{a} \tag{5}$$

The ratio $B_0/B_1$ is equal to the ratio of adhesive surface areas in each case. The area for coefficient $B_0$ is calculated as the total surface of $l$ individual filaments (with diameter $d$) in the yarn within a cubic cell (with side length $a$), assuming that filaments within a yarn are evenly packed and stretched straight along the axis of the yarn, and the area for coefficient $B_1$ is calculated as the area of the cell. The value of $B_1$ is determined by simulation to accommodate the experimental data. The values of $C$ and $B_0$ are determined by Eq. (5).

To test the validity of the model, a set of vertical wicking experiments were performed. Test samples included three types of weakly twisted polypropylene filament yarns with the same yarn count but different

Table 1
Specifications of PP yarn samples

| Sample | Yarn count (tex) | Diameter of yarn (mm) | Fineness of filament (dtex) | No. of filaments in a yarn | Diameter of filaments ($\mu$m) |
|---|---|---|---|---|---|
| 1 | | 0.282 | 2.25 | 60 | 18 |
| 2 | 13.4 | 0.290 | 1.5 | 90 | 14.6 |
| 3 | | 0.322 | 0.6 | 224 | 9.2 |

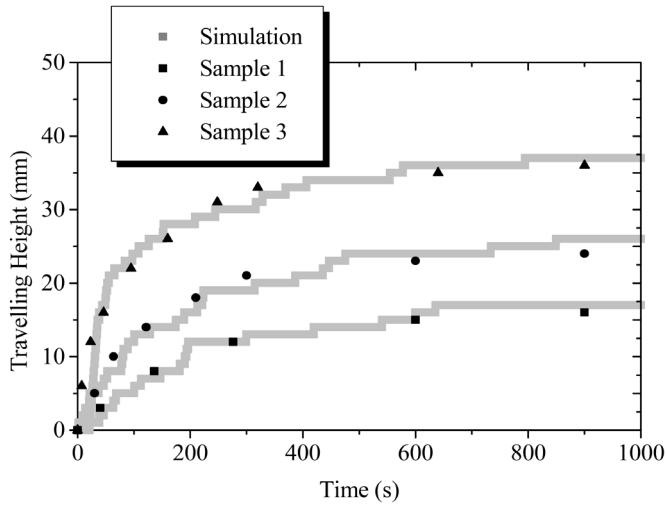


Fig. 1. Traveling height of liquid versus time.

fineness of constituent filaments. Their specifications are listed in Table 1. The experimental as well as the simulation results of the wetting rate are shown in Fig. 1.

Results of experiments and simulations show considerable agreement. Keeping the yarn count constant, but decreasing the yarn filament diameter, the total surface area of a unit length of the yarn increases, which in turn causes an increase in the interaction area of fiber and liquid, and thus in the interaction energy, resulting in a higher wettability of the yarn.

### 3.2. From statistical mechanics to macro properties of fibrous materials

Figure 2 shows a simulation of the dynamics of liquid wetting/wicking into a fibrous mass with varied fiber declination $\beta$ from the vertical axis: $\beta = 0^\circ$, $10^\circ$, $20^\circ \ldots$ $90^\circ$, plus $\beta = 45^\circ$. Each picture shows paired wetting patterns of a cross section with both side and top views.

The results show that, at $\beta = 0^\circ$, the ascending liquid moves at the highest rate but is mostly scattered; while at $\beta = 90^\circ$ it has the lowest wetting rate, but with the most heavily aggregated liquid.

To transfer these simulation results into macro parameters, such as liquid wicking rate, a modified version of the Lucas-Washburn equation is applied.

Classic Lucas-Washburn theory describes the liquid's velocity, $dh/dt$, moving up or down a perpendicular capillary with radius $r$:

$$\frac{dh}{dt} = \frac{r\gamma\cos\theta}{4\mu h} - \frac{r^2\rho g\cos\beta}{8\mu} \tag{6}$$

Several parameters included in the equation are contact angle $\theta$, viscosity of liquid $\mu$, surface tension $\gamma$, density of liquid $\rho$, and gravity $g$.

For a given system, the Lucas-Washburn equation (6) can be reduced and modified by introducing two constants [2]:

$$K = (wT\rho V_L)^2\frac{r\gamma\cos\theta}{4\mu}, \quad L = wTV_L\frac{r\rho^2 g\cos\beta}{8\mu} \tag{7}$$

which results in a simplified version:

$$\frac{dm}{dt} = \frac{K}{m} - L \tag{8}$$

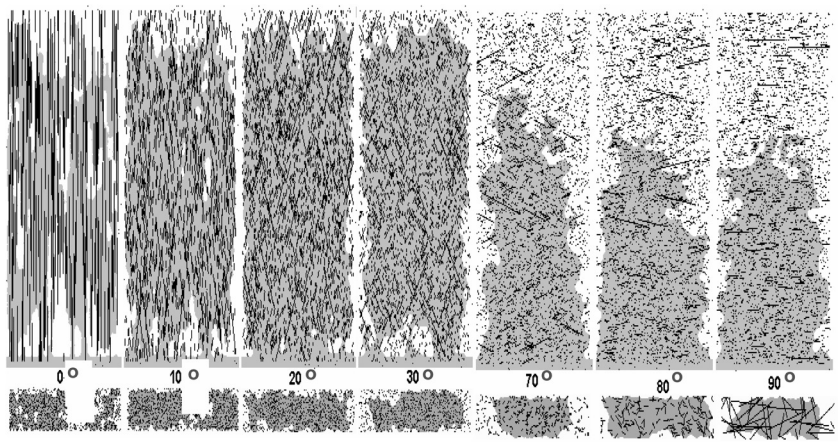


Fig. 2. Wetting patterns of a fibre mass with different $\beta$ after 600 MCS.

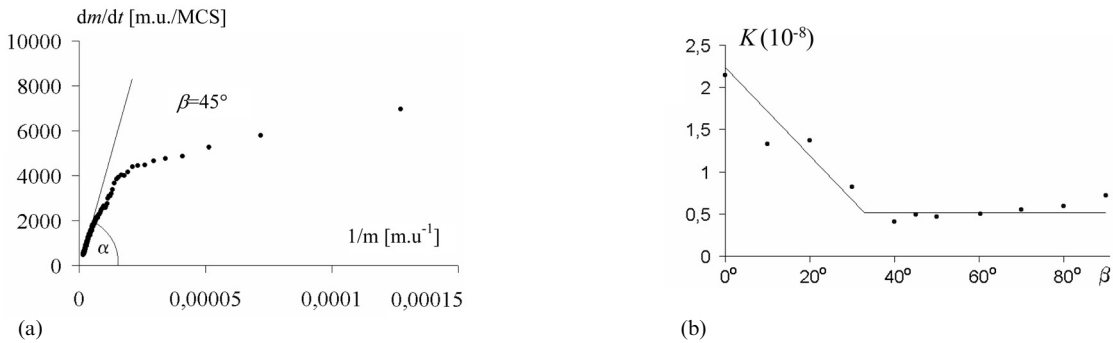


Fig. 3. The wicking rate vs. fiber orientation angle. (a) $dm/dt$ against the reciprocal of mass $1/m$. (b) $K$ against $\beta$.

The parameter $K$ can be used as a measure of the liquid wicking rate in a fabric hung vertically. The values of $K$ and $L$ can be derived from the slope and intercept of $dm/dt$ vs. $1/m$.

To evaluate the wicking rate $K$, $dm/dt$ is plotted against the reciprocal value of the mass $1/m$ with different $\beta$ values in Fig. 3(a). According to Eq. (8), $dm/dt$ against $1/m$ should be linear. The results of the simulation, which is consistent with experimental practice, demonstrate otherwise. Actually, $dm/dt$ cannot remain constant as gravity will reduce and eventually stop the wicking process. This again provides strong evidence for validating our computer simulation method.

An analysis of the relationship between wicking rate $K$ and the fiber mass orientation angle $\beta$ based on the simulated data is summarized in Fig. 3(b). The relation between them is also non-linear, with rapid decrease of $K$ in the interval $\beta \in \langle 0^\circ, 30^\circ \rangle$, while at $\beta > 30^\circ$ it shows a constant or even slight increase of $K$.

## 4. Conclusion

A multi-scale modeling of transport in fibrous materials is reported in this paper, going through from quantum field theory, to statistical mechanics, and then to classical continuum methods. The transition from one scale to another is carried out by a so-called 'hand-shaking strategy', that is, the information gained from a lower scale is summed into a finite set of parameters, and passed onto the higher scale. Specifically, the Hamaker constant, which is required as an input for Ising's model, can be calculated from quantum field theory. Then, the predicted transport behavior of liquid in fibrous materials can be used in a modified version of the Lucas-Washburn equation to give the wick rate of a specific fibrous structure. The simulation agrees well with experimental results, indicating the useful power of this approach in the application of similar micro- and nano-mechanics of materials.

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