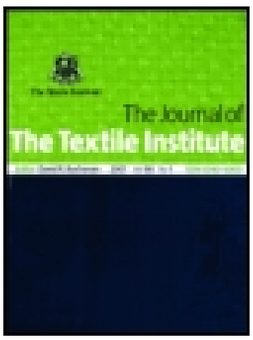

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Computer Simulation of Liquid Wetting Dynamics in Fiber Structures Using the Ising Model

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We present in this paper a method which applies the so-called Ising model and Kawasaki thermodynamics, combined with the Monte Carlo computer simulation technique to study the liquid-fiber interaction and the wetting behavior of fiber networks.

The various types of interactions occurring during a wetting process in a fiber mass are analyzed, and their individual contributions towards the Hamiltonian system are derived. The criterion for energy state exchange between the Ising spin variables is given as the critical step for the wetting simulation.

The procedures of the simulation algorithm are provided. Various predictions of the wetting process including wetting of a fiber network, the spreading of a liquid drop on a single fiber as well as a brief parametric study are included in this paper.

1. INTRODUCTION

The wetting of a fiber mass is an important issue in a range of areas including textile and composite manufacturing. In textile applications we can mention, for example, sports clothes, hygiene disposable materials, medical products, and geotextiles where the wetting behavior of the fibrous structures is a critical aspect of the performance of the products. In addition, the wetting process occurring especially during dyeing, finishing and the wearing of clothing all have a practical significance in controlling the quality of the textile processing and the clothing comfort. Another example where the wetting process is considered extremely important is in the application of fibrous filters, where competitive wetting of the fiber surface is the key mechanism for the separation of two different liquids from their mixture, for instance, the separation of oil from sea water during a cleaning process after an oil spillage.

Therefore, extensive wetting research work has been undertaken in the area of textiles. A classic theory of wetting through capillary dynamics was proposed by Washburn in 1921. New advances have been made in recent years as well. Wehner *et al.* (1988) developed a new experimental apparatus for the simultaneous measurement of moisture sorption by a fabric and moisture flux through a fabric during the transient period after the fabric is exposed to a humidity gradient, and based on the experimental measurements, a theoretical model is presented. The dynamic process of water vapor and heat transport in textiles have been dealt with by Wang and Yasuda (1991), by Kim and Spivak (1994), and by Yasuda *et al.* (1994) reported in a three-part series paper in which the effects of fiber properties, layers of fabrics, and the structure of fabrics on the transport process are studied experimentally in great detail. Hsieh and colleagues (1992, 1995) have also developed an experimental protocol for the measurement of liquid wetting and retention characteristics

in woven fabrics with an extensive experimental and theoretical analysis.

In the composite fabricating process, the matrix of the liquid phase is poured on and allowed to penetrate a fiber preform. Thus, understanding how the liquid interacts with or wets the fibers will provide crucial information on how to improve the quality of the fiber reinforcing effects. Kim and colleagues have investigated the resin flow behavior in a fiber preform during composite processing (1991). Castano *et al.* (1992) have studied the resin-fiber interaction in an attempt to fabricate a composite reinforced by natural fibers (1992). Skartsis *et al.* (1992) have treated the liquid resin as a Newtonian fluid so that fluid mechanics is applied to simulate the flow behavior of the resin (1992). More recently, Patel *et al.* studied the interactions at the resin-fiber interface (1993).

In spite of the practical importance of the liquid and fiber mass interaction, most theoretical papers on the wetting phenomenon are devoted to solid planar surface wetting, following the pioneering work of Young and Laplace (1805). As can be seen in the next section, there are a number of important differences between wetting a solid planar surface and a fibrous structure. The present paper is an attempt to apply the Ising model combined with the Monte Carlo simulation to the study of the wetting behavior of a fibrous substrate. It is our hope that through this paper we will be able to predict the dynamics of the wetting process of a fibrous structure and hence demonstrate the usefulness and power of the Ising model in this area.

The so-called Ising model proposed by Ising in 1925 was initially used as a tool to study ferromagnetic phase transition. It was later found that it could also be used as a powerful model for the investigation of several other physical phenomena such as liquid-gas transition (McCoy and Wu, 1973) and the order-disorder transition of alloys (Onsager, 1944). In recent years, with greater attention being paid to the wetting process, the Ising model has been proved to be a potent technique in the wetting mechanism study. A series of papers have since been published by Binder, Landau, and colleagues (1988;1989;1990;1991;1992), and other researchers (Gompper *et al.*, 1990; Abraham and Newman, 1988; Kaski, 1995) on the investigation of the wetting process and related problems by using the Ising model.

2. THERMODYNAMICS OF THE ISING MODEL FOR LIQUID-FIBER INTERACTIONS

In this section, we will first introduce the various interactions occurring in a liquid-fiber mixture and the energy components associated with these interactions. Then a criterion of state change according to Kawasaki dynamics (Manna *et al.*, 1992) is established as a mechanism describing the liquid-fiber wetting dynamics. Finally, the Monte Carlo stochastic approach is employed to simulate the liquid wetting process.

2.1 Unique Features and Problems of Fiber Wetting

As pointed out above, the previous wetting researches have been mostly focused on the solid planar surface. It is therefore necessary to point out the differences in wetting a solid plane and a fiber mass:

1. A fiber mass is, as a rule, heterogeneous and anisotropic. That is why the resultant mechanism of interactions with liquid is more complex, compared with the solid planar case.
2. A fiber is not straight in general, and ideally has a value of mean curvature equal to $1/2b$ where b is the fiber's radius, while the mean curvature for a plane is 0 (Saxl, 1989). The consequence of this leads to the different conditions for the complete wetting in these two cases.

Brochard (1986) and Bacri (1988) have dealt with the problem of single fiber wetting where a fiber of radius b is covered by a layer of liquid film with the equilibrium thickness e_0 (see Fig. 1). They used the spreading coefficient S (De Gennes 1985) to express explicitly the aforementioned differences.

$$S = \gamma_{so} - \gamma_{sl} - \gamma_{ll} \tag{1}$$

where γ_{so}, γ_{sl}, and γ_{ll} represent the surface tensions of the solid, the solid-liquid interface, and the liquid, respectively. Then the complete wetting of the fiber occurs when

$$S \geq 0 \tag{2}$$

This condition for a fiber was eventually changed into another inequality

$$S \geq e_0/b$$

Equation (1) is useful for understanding the liquid-fiber interactions during the wetting process. The three types of interactions in the equation will be discussed in detail below in order to formulate the theoretical frame of the present work.

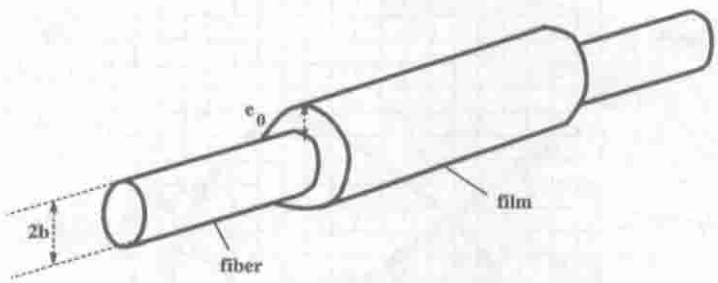


Fig. 1 A fiber of radius b covered by liquid film of equilibrium thickness e_0

To begin with, we will introduce a simple computer simulation method based on the two-dimensional Ising model in this paper. For a two-dimensional case, the issue of fiber curvature discussed above becomes irrelevant and the model will only exhibit the heterogeneous and anisotropic features of a fiber network. The base for the present study is the work by Manna, Hermann, and Landau (1992) that deals with the motion of a liquid drop on a wall.

2.2 The Ising-system Spin Variables

According to McCoy and Wu (1973), a two-dimensional Ising model consists of a lattice of 'spin' variables σ_i, which can only take the value +1 or –1. Any two of these 'spins' will have a mutual interaction energy as follows:

$$H_i = H_j = E(\sigma_i, \sigma_j) \tag{4}$$

The meaning of this definition is that the mutual interaction energy H_i belongs to the cell i with the spin variable σ_i. This energy is negative when σ_i and σ_j are both +1 or –1, the two spins then attracting each other, but is positive when σ_i and σ_j have opposite signs with a repulsion situation existing between them.

In addition, a spin σ_i may interact with an external gravitational field G_y with an energy of:

$$H_g(i) = E_g(\sigma_i, y_i) \tag{5}$$

where y_i is the vertical coordinate of the cell i in the field. Similarly, the interaction energy is negative or positive depending on the sign of the spin σ_i.

For our problem of liquid-fiber mass wetting, we begin with a finite two dimensional regular and square lattice of cells (see Fig. 2). Each cell is denoted by the index i and is occupied by either of the two fluids (liquid or air). We can therefore use the spin variable of the Ising model: the spin $\sigma_i = +1$ when a cell is filled by the liquid, whereas $\sigma_i = -1$ means the cell is filled by air or, simply, is an empty cell.

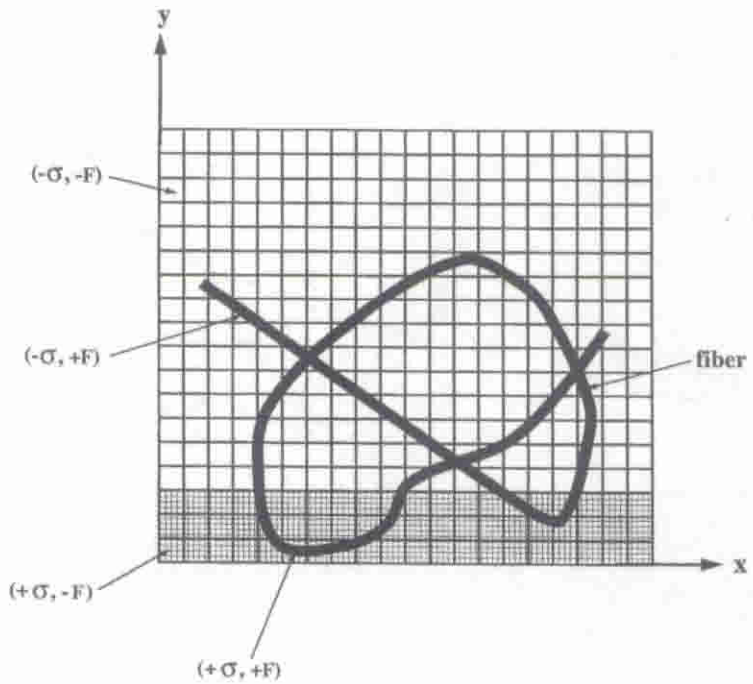


Fig. 2 The co-ordinate system, the lattice and various spin cells

Furthermore, in order to incorporate the fiber network into the system, the cells of the lattice can also be occupied by the fiber substrate for which a second kind of Ising spin variable F_i is defined. Cells occupied by fibers have the variable $F_i = +1$, or alternatively $F_i = -1$.

The spin variables σ and F can overleap in each lattice cell, meaning that a cell may be occupied simultaneously by the fiber material and one type of the fluids of either the liquid or air as illustrated in Fig. 2, where the shadowed cells indicate the cells filled with liquid, and the blank ones are filled with air, and a fiber is laid on the lattice, sharing the cells with either the liquid or air.

During the computer simulation process, the fluid Ising variables or the cells can interchange their positions, reflecting the movement of liquid during the wetting process,

but the fiber spins are stationary.

If this system with overlapped cells is then placed into an external field of gravitation with gradient G_g, as is the case with Equation (5), three types of interactions will occur in the system, i.e.,

- interaction of the cells with the external gravitational field;
- interaction among the fluid cells, a reflection of the liquid surface tension and liquid–liquid cohesion; and
- the adhesive interaction between the cells of the fluids and the fiber substrate.

Each type of interaction contributes to the total energy (the total Hamiltonian) of the whole system, and the dynamics of the fluid mixture are governed by the thermodynamic rules.

2.3 Description of the Energy Contributions

We now calculate the energy contribution below for each type of cell interaction. The total energy of the system is then given as a sum of all the contributions of the cell energies in the lattice.

2.3.1 Energy of a Fluid Spin in the Gravitational Field

The magnitude of the gravitational energy, $H_g(i)$, of a cell i occupied by a fluid increases proportionally along the y abscissa of the lattice in Fig. 2, i.e.,

$$H_g(i) = G_g \sigma_i y_i \tag{6}$$

where G_g is a constant.

Note that, since the cell i can take $\sigma_i = 1$ or -1 depending on whether the cell is filled with liquid or air, $H_g(i)$ can be either positive or negative.

2.3.2 Interaction Among the Fluid Spins

The spin-spin interaction between the fluid cells occurs only among the cells within a certain proximity to each other, if we consider that the influence of the remote cells is negligible. More specifically, let us assume that we only need to account for three types of neighboring cells in terms of closeness, denoted as the nearest neighbor, the next nearest neighbor and the next-next nearest neighbor. The interaction energy for a liquid cell i can be calculated by using the following equation:

$$H_c(i) = -\left(C_1 \sum_j^n \sigma_i \sigma_j + C_2 \sum_j^{nn} \sigma_i \sigma_j + C_3 \sum_j^{nnn} \sigma_i \sigma_j \right) \tag{7}$$

where the C_i's are the positive constants. The first term in this equation is the sum of all the nearest neighbors, the second one over the next neighbors, and the third figure is the one over the next-next neighbors. This kind of energy interaction represents the effects associated with the surface energy and surface tension between the liquid filled cells, and can hence be treated as the cohesive energy. The three types of cells are sketched as three different layers surrounding the selected cell i as seen in Fig. 3(*a*) where the three types of cohesive interactions are divided into three layers denoted as the first, second and third layer. The first layer consists of the cells of the nearest neighbors (n) associated with the constant C_1. Similarly, the second and third layers represent the cells of next nearest (nn) and next-next nearest (nnn) with interaction constants C_2 and C_3, respectively.

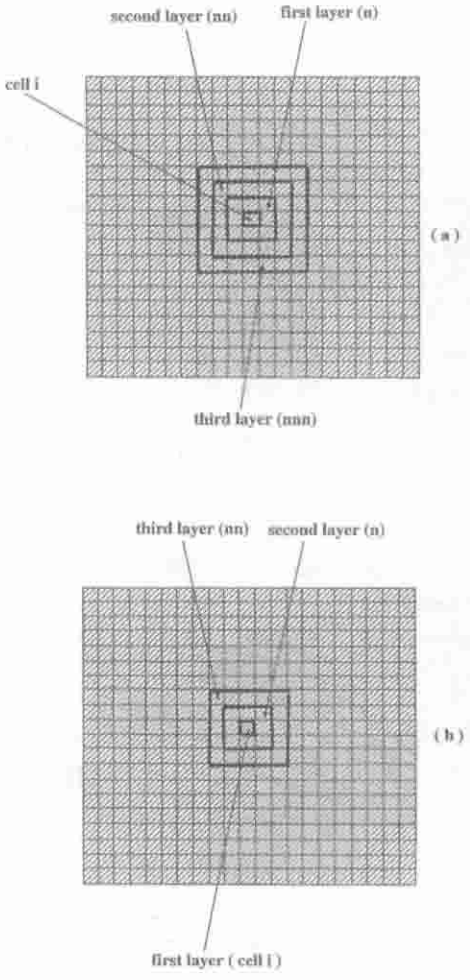


Fig. 3 The ranges of the interactions: (*a*) the cohesive interactions; (*b*) the adhesive interactions

2.3.3 Interaction Among the Fluid and the Fiber Substrate Spins

The last part of the Hamiltonian system consists of energy terms generated from the fluid–fiber interaction, which reflects the adhesive forces. A cell i occupied by fluid interacts with the following three types of fiber cells:

- overlapped cells by the fluid and the fiber substrate;
- the nearest-neighbors fiber cells; and
- the next-nearest neighbors fiber cells.

The sum of the above three types of energy contribution is:

$$H_a(i) = -\left(A_0 \sigma_i F_j + A_1 \sum_j^n \sigma_i F_j + A_2 \sum_j^m \sigma_i F_j \right) \tag{8}$$

Again, A_i's are positive constants associated with the properties of the fiber and the liquid. Likewise, the three types of adhesions are illustrated in Fig. 3(*b*) which shows the three

layers described above and includes the overlapped cell i of the fiber and the liquid. The first layer describes the interaction reflected by the coefficient A_0 between the fiber and the liquid in this overlapped cell, and the nearest neighbors are in the second layer (n) whose interactions with cell i are represented by A_1, just like the next nearest layer (nn) represented by A_2.

Then the total Hamiltonian of the lattice model is as follows:

$$H = \sum_i \left[H_s(i) + H_c(i) + H_w(i) \right] \tag{9}$$

The magnitude of this total Hamiltonian is the source for the system wetting dynamics.

2.4 The State Probability and the Kawasaki Dynamics

Let us consider the Ising model as a thermodynamics system connected with a thermodynamics reservoir, and energy exchange can occur between them. The system together with the reservoir forms a canonical assembly that is governed by the Boltzmann distribution of the state probability ratio

$$\frac{P(H_1)}{P(H_2)} = \Lambda = \exp\left(-\frac{1}{\tau} \Delta H \right) \tag{10}$$

where the parameter τ is proportional to the absolute temperature, and Λ is the ratio of $P(H_1)$ and $P(H_2)$, $P(H_k)$ (where k =1 and 2) being the probability that the system exists with configuration associated with energy H_k. The parameter Λ is then a measure of the likelihood for the system to change its configuration, through spin exchange, from the state with energy H_1 to the state with energy H_2. The energy difference $H_1 - H_2$ denoted by ΔH is the difference of the total system energy before and after the spin exchange. The dynamics is realized by a spin exchange that occurs over distances and this kind of dynamics is in the literature described as Kawasaki dynamics (Manna *et al.*, 1992). Two cells are randomly chosen on the interface between fluid and air. One of them has the spin variable $\sigma_i = +1$ and the other $\sigma_j = -1$. A random number $r \in [0,1]$ is then generated. In the case where r is less than the probability for spin exchange that is given by the Boltzmann law, i.e.,

$$r < \Lambda = \exp\left(-\frac{1}{\tau} \Delta H \right) \tag{11}$$

these two spins will exchange their position.

The implication of the connection between the energy state and the spin exchange probability in Equation (11) is very important. Since the probability ratio cannot be greater than 1, so the case where $\Delta H < 0$ is not viable, no spin exchange will occur under this condition since it represents a transition from a more probable spin configuration to one with a lower probability. When $\Delta H = 0$ so that $\Lambda = 1 \geq r \leq 1$, the spin exchange is possible but with a very small probability (only occurring when $r = 1$). Whereas when $\Delta H > 0$ and $r \leq \Lambda < 1$, spin exchange is encouraged and most likely to occur as illustrated in Fig. 4.

3. TREATMENT OF THE FIBER ORIENTATIONS

The fiber assembly for the wetting simulation is created in the following way. The fibers are considered straight and identical in length and radius, and both values as well as the total fiber number are given as the input parameters for simulation.

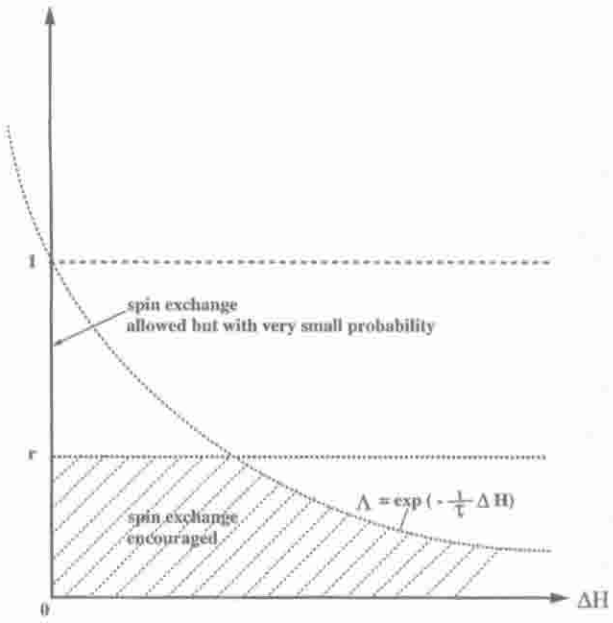


Fig. 4 Illustration of the spin exchange criteria

The distribution of fibers in the Ising model lattice are specified by using the center along a fiber length as the location parameter, and, for the planar fiber network case, by using an angular variable $0 \leq \phi \leq \pi$ as the direction parameter defined as the angle of the fiber with respect to the vertical direction y. In the following simulations, we assume a fiber mass where all fibers are randomly oriented so that the individual fiber direction ϕ in a lattice is decided by means of a random number generator.

A lattice cell i is considered to be occupied by a fiber (i.e., $F_i = 1$) when the distance between the cell center and the fiber axis is smaller than the fiber radius.

4. THE COMPUTER ALGORITHM PROCEDURES DEVELOPED FOR THE MODEL

The procedures of the computer algorithm developed for this simulation process contain four major steps and a final action.

1. Creating the initial configuration – this includes the development of the lattices, on top of which a fiber network, based on the given fiber orientation, is laid. The initial conditions are set so that the original state of each cell (the spin) is determined – for instance, the cells at the bottom are initially filled with liquid.
2. Scanning the liquid–fiber interface. Each pair of cells of spins σ_i and σ_j is randomly scanned – one pair being filled with liquid and the other with air – the Hamiltonians H_1 and H_2 are calculated for cases before and after the spin exchange, and determining the Λ value according to Equation (10).
3. The generation of a random number r.
4. The two spins σ_i and σ_j are exchanged if Equation (11) is satisfied.
5. Finally, stop if the system has reached a certain equilibrium judged by a given criterion – for instance, when the liquid height no longer rises with time. Otherwise go back to Step 2.

5. OUTPUTS OF THE COMPUTER SIMULATIONS

A computer simulation software based on the above procedures has been developed for the fiber network wetting process. One result of the liquid wetting simulation in a fiber network is shown Fig. 5. The fibers as mentioned earlier are considered as randomly distributed. For the simulation, the following values are chosen for all the unknown constants:

$$G_g = 1,\ C_1 = 30,\ C_2 = 20,\ C_3 = 10,\ A_0 = 15,\ A_1 = 10,\ A_2 = 5,\ \tau = 4;$$

The simulation was terminated after 500,000 spin exchanges for a lattice size of 175 × 350 cells. It is seen that at different times t of an artificial unit defined as the period for 1000 trials of spin exchange, the liquid is gradually wetting the fiber network, and the liquid films on and between the fibers are observed in Fig. 5(*a*). The height of the liquid front in the fiber network increases with time as shown in Fig. 5(*b*) where again the numbers are in relative units.

For different sets of the parameters, the wetting behavior shows different patterns as illustrated in Fig. 6 where Cases A, B, and C are represented by the following:

(A) $G_g = 1,\ C_1 = 30,\ C_2 = 20,\ C_3 = 10,\ A_0 = 15,\ A_1 = 10,\ A_2 = 5,\ \tau = 4;$
(B) $G_g = 1,\ C_1 = 30,\ C_2 = 20,\ C_3 = 10,\ A_0 = 30,\ A_1 = 20,\ A_2 = 10,\ \tau = 4;$
(C) $G_g = 1,\ C_1 = 10,\ C_2 = 5,\ C_3 = 2,\ A_0 = 60,\ A_1 = 40,\ A_2 = 20,\ \tau = 4.$

The three cases in the figure are the results obtained after the same time period. Case B has the same conditions as Case A except that the adhesive interaction between the fiber and the liquid is stronger which is reflected by the doubled A_i values, i.e., there is a closer affinity between the fiber and the liquid. As a result, the liquid wets the fiber network faster in Case B than in Case A. Whereas in Case C, the cohesion between the liquid is weaker judging from the smaller C_i values and the adhesion between the fiber and the liquid is even greater, leading to an even quicker wetting process.

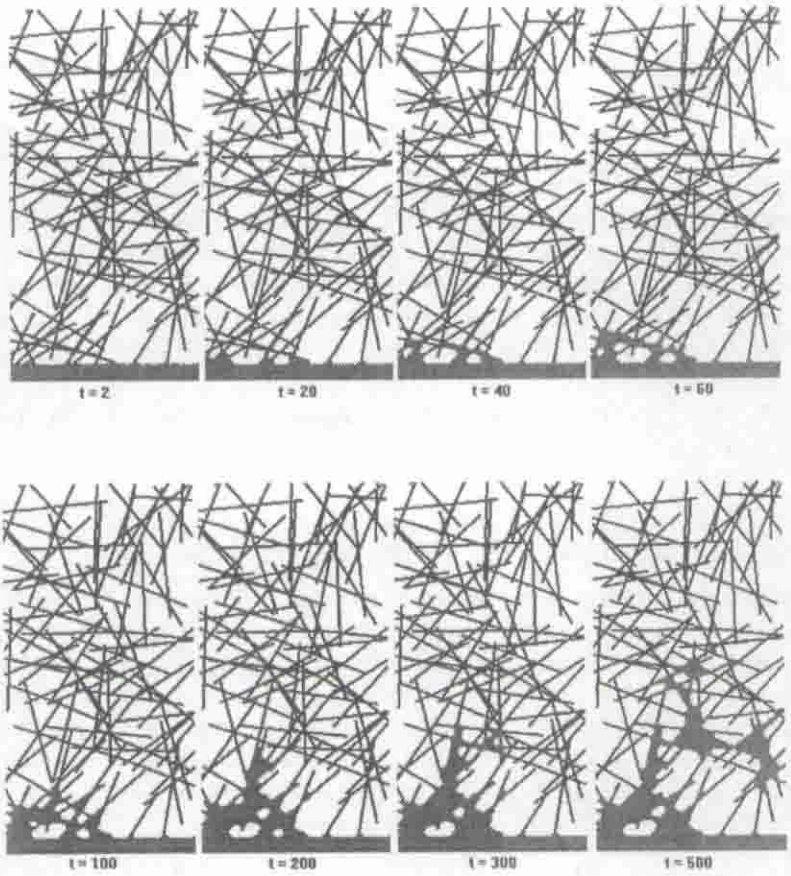
Finally, by using the following set of the parameters:

$$G_g = 1,\ C_1 = 30,\ C_2 = 20,\ C_3 = 10,\ A_0 = 15,\ A_1 = 10,\ A_2 = 5,\ \tau = 4$$

we carried out the computer simulation of the dynamic process of spreading a liquid drop on a fiber, and the results are provided in Fig. 7, depicting the changing shape of the liquid drop after seven different time periods.

From the above simulation theories and the examples, several advantages can be found about the present approach. Firstly, the Ising model can describe a complex physical phenomenon in a very simple binary form, yet can still be able to account for all the mechanisms involved, and yield realistic results. This makes the model a very attractive, practical and powerful tool to study wetting phenomenon. Also, the constants associated with the energy terms have very clear physical meanings, and they in fact represent the properties of the medium involved. Thus, by adjusting the values of these constants, we can carry out a series of parametric studies of the influences of these properties on the problem under investigation.

In addition, the examples of simulation provided above are for illustration purposes only in order to show the usefulness of the present method, and many more applications of this method can be explored. For instance, by changing the temperature-related coefficient τ, the temperature effects can be studied. More complex problems, such as those with irregular lattices and three-dimensional cases can also be studied in a similar fashion. For a more realistic simulation of practical fibrous structures, experimentally determined fiber distribution characteristics such as those given by Huang and Breese (1993) and Saxl and Rataj (1988) should be used. These issues will be dealt with as a continuation of this research work.



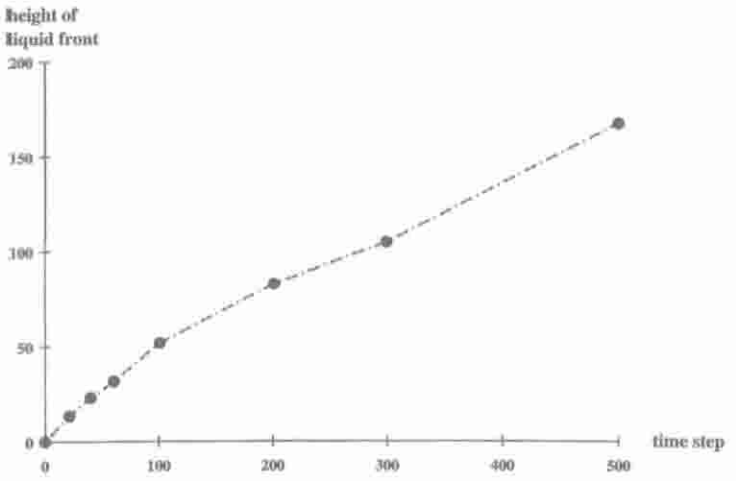


Fig. 5 The wetting simulation results in relative units: (*a*) Wetting progress with time in a fiber network; (*b*) Change of the height of the liquid front during wetting

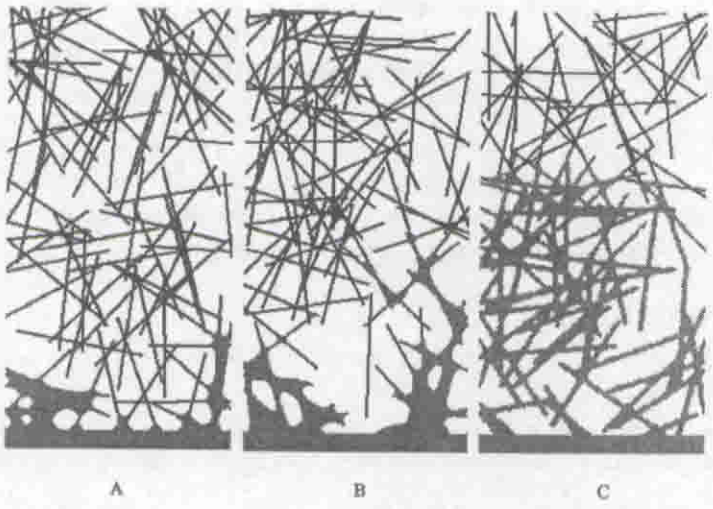


Fig. 6 Wetting processes with different system parameters

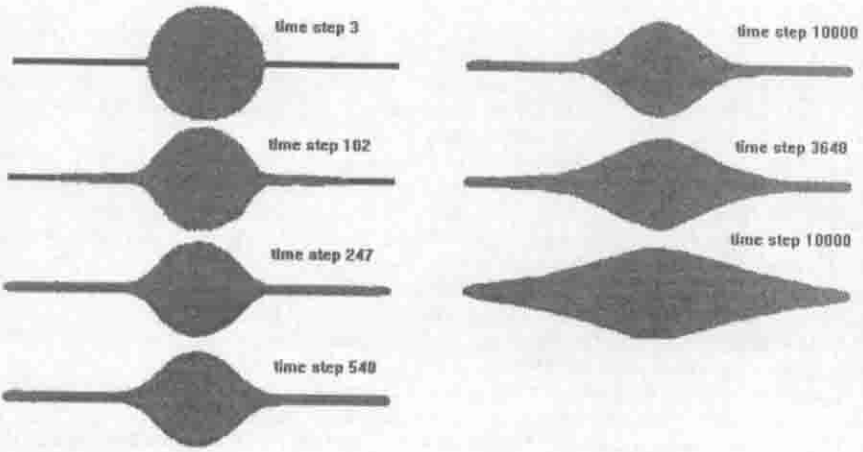


Fig. 7 Simulation of the spreading of a liquid drop on a fiber

6. CONCLUSION

The result of this paper is the stochastic computer simulation of liquid-fiber interactions. One of the advantages of the present method is its simplicity in application. A very complex wetting process can be realistically simulated without employing intricate mathematical models.

The proposed simulation technique enables us to obtain information about the nature and mechanisms of the fiber mass wetting behavior. All the important interactions and factors have been included in terms of the energies they contribute to the whole process. The results obtained are in good qualitative agreement with the behavior of real systems. This model has demonstrated its power in studying various wetting problems for practical applications.

Some improvement can be made on the present model. Irregular lattices can be used to replace the regular one used in this study, and the model can be expanded into three-dimensional cases so that problems in practical fiber structures can be examined.

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