

Analysis and modelling of wicking through carton liquid packaging

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Abstract

One of the more important issues in carton liquid packaging systems is the wicking of liquid content through the carton (usually coated with polymeric films) packaging. A suitable carton packaging for liquid content should have slow rate of wicking to provide satisfactorily long shelf life of the packaged product. In this study, the phenomenon of wicking of various liquid products, through coated carton packaging, was investigated. Thus, methods for the analysis of wicking through carton packaging had been developed. Mathematical models relating the rate of wicking to the physical–chemical properties of the liquid content and of the carton board were proposed. Model parameters for a widely used carton packaging material were obtained based on experimental data. The models obtained were proven capable of giving reliable correlation of the rate of wicking to the physical–chemical parameter of the liquid content and of the coated carton packaging. © 2005 Elsevier B.V. All rights reserved.

Keywords: Wicking; Diffusion; Particle size analysis; Modelling of wicking; Carton packaging

1. Introduction

Cellulose based materials have long been used as more environmentally friendly materials for packaging. Worldwide, the total weight of cellulose based packaging materials used is similar to the total weight of all other packaging materials used [1,2]. Recent development in the polymeric coatings for carton boards has made it possible to use carton board in the packaging of liquid products. One of the difficulties in selecting suitable coated carton board for the packaging of liquid products is the large variety of the liquid products. Each liquid product to be contained in carton packaging has its own unique chemical and physical–chemical properties. It was demonstrated, in a previous publication [3], that the nature of wicking through liquid packaging systems is significantly influenced by the viscosity, the particle size and size distribution and the surface tension of the liquid content.

From the point of view of the packaging industry, suitable approaches for the rapid evaluation of the suitability of coated carton materials for the packaging of liquid products are desirable. Currently, in order to evaluate the suitability of a coated carton packaging material for a particular liquid content, laboratory tests, i.e. wicking test, have to be carried out to establish the rate of wicking of the liquid product through the carton packaging material. Such tests are relatively time-consuming, which is particularly true considering the fact that a significant number of parameters of the carton material are of concern. Such parameters include the thickness of the carton, the thickness of the polymeric coating, the chemical resistance of the polymeric coating, the barrier properties of the polymeric coating. The wide variety of the liquid content adds significant complexity to the problem.

Therefore, a mathematical model accurately describing the relationship between the rate of wicking and the various physical–chemical properties of the polymeric coating, of the carton board and of the liquid product is desirable. Using such a model, rapid evaluation of the suitability of the coated carton for packaging for a particular liquid containment can be made.

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Carton boards, being cellulosic in nature, have considerable affinity to aqueous liquids, such as fruit juices, detergents, paints, etc. Consequently, wicking becomes one of the major problems in liquid packaging. To alleviate the extent of wicking, carton boards are usually coated with a polymeric film to improve the barrier property. Typical polymers used for such purpose include poly(ethylene), ethylene-vinyl alcohol copolymers and poly(propylene). Such polymeric barrier coatings also need to be chemically resistant to liquid containment. Details of the effects of the liquid products on the polymeric coatings have been published elsewhere [4].

2. Preparation of carton packaging for liquid containment

For the purpose of forming desirable container, the coated carton boards have to be subjected to die-cutting, die-creasing, erecting, and sealing (usually by heating). A typical carton package and relevant die-cutting and creasing pattern are schematically illustrated in Fig. 1.

In the production process, the creased and cut flat cartons are folded to form a three-dimensional structure that is strengthened by heat sealing. The folding and heating processes are likely to cause damage to the polymeric coating thus creating fractures and pinholes. In the packaging shown in Fig. 1, the corners of the triangle flaps are usually subjected to most mechanical and thermal disturbance (Fig. 2).

There are also likely to be pinholes in the polymeric film coated on the carton base. In practice, it is often inevitable that the liquid content migrate into the carton through either the pinholes or the cracks in the coating in contact with the liquid product (usually the inside of the packaging). The liquid product will then continue to travel through the carton base, usually along the grain direction. The liquid product will eventually emerge from the other side through pinholes or crack in the polymeric film coated on the other side of the packaging. It should be emphasised that the most likely route of migration of the liquid product is that along the grain direction, a fact that has been established previously [4].

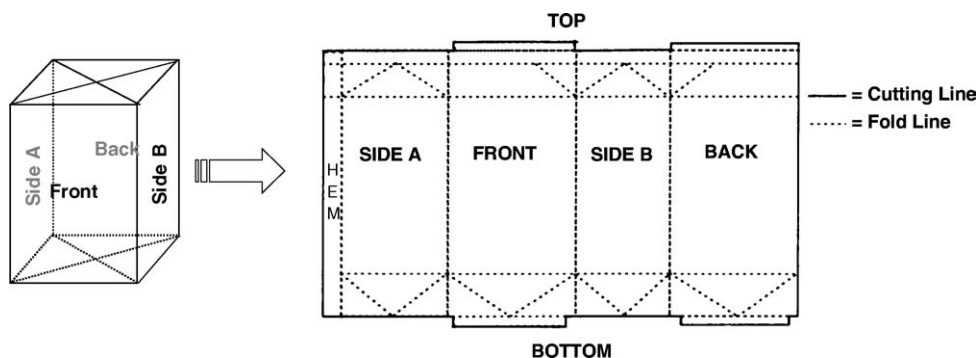
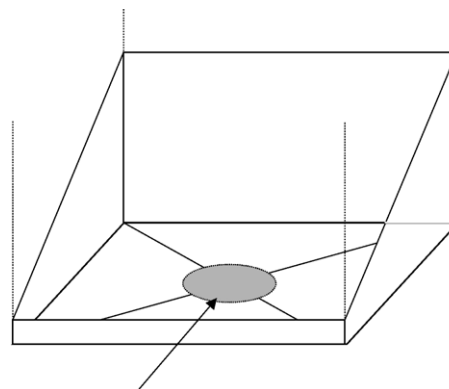


Fig. 1. A carton package and relevant die-cutting and creasing pattern.



Corners of the triangular flap

Fig. 2. The corners of the triangle flaps where most mechanical and thermal disturbance occurs.

3. Modelling and prediction of wicking—the concept

3.1. Establishment of mathematical models

Mathematical modelling of diffusion of liquid and gas through polymeric barrier materials has been reported elsewhere [5–8]. Various models have been developed to simulate the diffusion of moisture through cellulose based packaging materials [9–14].

In particular, several models have been developed for the sorption and diffusion of moisture through heterogeneous media, such as paper and carton [15–21]. However, there exist very few reports on sorption and diffusion of liquid containing particles, such as detergents and fabric conditioners. Thus, mathematical models for the simulation of the relationship between the rate of wicking and the physical–chemical parameters of the coated carton board and of the particulated liquid content needed to be established. In this study, only the flow in the direction of the grain of carton board was considered. This was because that the rate of diffusion across the grain was usually relatively insignificant, comparing to that along the grain. As such, the structure of the carton board can be considered as porous medium consisting of a bundle of cylindrical capillary tubes.

Assuming quasi-steady creeping flow, wicking phenomena is commonly described by the theory developed by Lucas [22] and Washburn [23]. Thus, the relationship between the rate of wicking and the physical–chemical properties of the carton board and of the liquid can be simulated using Eq. (1):

$$h = \left(\frac{\rho\sigma \cos \theta}{2\tau^2\mu} \right)^{1/2} t^{1/2} \quad (1)$$

where h is the nominal distance travelled by the liquid, τ an appropriate tortuosity factor of the carton board, μ and ρ the liquid viscosity and density, respectively, θ is the dynamic advancing contact angle of the liquid on carton board, and σ is the liquid surface tension.

From Eq. (1), it can be seen that the rate of wicking is proportional to the square root of time, for any individual carton board/liquid assembly. Consequently, for any individual liquid, weight gain of the carton board due to the wicking of liquid, W , should also be directly proportional to the square root of time elapsed, by a factor of W_0 , as shown in Eq. (2):

$$W \propto W_0 t^{1/2} \quad (2)$$

where

$$W_0 = \left(\frac{\rho\sigma \cos \theta}{2\tau^2\mu} \right)^{1/2} \quad (3)$$

It can be seen, from Eq. (3), that W_0 is a function of the physical–chemical properties of the carton board and of the liquid contained. For convenience, W_0 is termed wicking coefficient throughout this paper.

To this point, it has been established that the weight gain of the carton board, as a result of wicking of the liquid contained, is proportional to the square root of the time of contact between the carton board and the liquid contained. However, it has to be pointed out that the Lucas–Washburn theory was intended to describe wicking phenomenon involving particle-free liquids. As most liquid detergent contains particulate matter of significant size, modification to the wicking model, represented by Eq. (3), was needed.

Based on past experience [4], it was clear that the rate of wicking of liquid detergent through carton board is determined by several factors including viscosity, density, surface tension and particle size distribution of the liquid detergent and the physical–chemical properties of the carton board. Thus, the following model (Eq. (4)) was proposed to simulate the relationship between the wicking coefficient, W_0 and the physical–chemical properties of the liquid contained, i.e. σ , ϕ , ρ and μ :

$$W_0 = c_1 \sigma^{c_2} \phi^{c_3} \rho^{c_4} \mu^{c_5} \quad (4)$$

In Eq. (4), ϕ is the particle size characteristics of the liquid detergent and c_1 – c_5 are the constants whose values are determined by the physical–chemical interactions between the liquid detergent and the carton board. All other symbols have the same significance as defined previously. Clearly, each liquid detergent will have a unique set of parameters, σ ,

ϕ , ρ , and μ , representing its physical–chemical properties relevant to wicking phenomenon. On the other hand, each carton board will have a set of unique constants, c_1 – c_5 , representing its physical–chemical interactions with liquid detergent, resulting in various degrees of wicking.

3.2. Model acquisition and prediction

To this point, it is clear that the essence of the proposed modelling and prediction approach is two-folds, namely:

- to define any liquid detergent by a unique set of parameters including σ , ϕ , ρ , μ and
- to define the barrier properties of the carton board (against liquid detergent migration) by a unique set of parameters c_1 – c_5 .

For any individual liquid detergent, the parameters σ , ϕ , ρ and μ could be obtained through laboratory analysis. The parameters representing the barrier effect of any individual carton board, i.e. c_1 – c_5 , could be obtained via the following procedures:

- select several liquid detergents of various physical–chemical nature, i.e. σ , ϕ , ρ , μ ,
- select the carton board of interest,
- carry out laboratory tests to acquire the rate of wicking of each liquid detergent (details of testing procedures are given later), represented by weight gain of the carton board after being in contact with the liquid detergent, and
- compute the coefficients c_1 – c_5 , by numerical optimisation or least-square fitting of Eq. (4).

At this point, a model simulating the rate of wicking of the liquid detergents through the carton board investigated, Eq. (5), could be obtained:

$$W = c_1 \sigma^{c_2} \phi^{c_3} \rho^{c_4} \mu^{c_5} t^{1/2} \quad (5)$$

Using Eq. (5), the rate of wicking of any liquid detergent, through any carton board, could then be predicted since parameters such as σ , ϕ , ρ , μ , and c_1 – c_5 were available. One of the advantages of such a model was that the value of the coefficients c_1 – c_5 was unique to individual carton board thus independent of the liquid detergent. In other words, provided that the values of the coefficients c_1 – c_5 for a type of carton board were available, the rate of wicking of any liquid detergent (recognised by the model as a set of parameters σ , ϕ , ρ , μ) could be predicted using Eq. (5).

4. Experimental

4.1. Materials and equipment

Investigation of the migration phenomenon and of the rate of migration was carried out using six commercial

liquid detergents, hereafter known as DI–D6, and one type of carton board, all supplied by Field Group, Killingworth, Newcastle Upon Tyne, UK. It should be pointed out that the current paper was intended to report a methodology, rather than a complete set of models, for the prediction of wicking of liquid product through carton packaging. As such, only one type of carton board was investigated. The method reported could be used to predict wicking behaviour of other types of carton board. From the point of view of board structure, there are only a limited number of different carton boards in commercial use. Therefore, a library of models for the prediction of wicking for most commercially available carton boards could be established with relative ease.

The physical–chemical properties of the liquid detergents were analysed. Such physical–chemical properties included the density, the surface tension, the viscosity and the particle size and size distribution. The procedures for the determination of these properties and of the rate of wicking are detailed as follows.

4.2. Procedure for the measurement of the specific gravity of the liquid

The specific gravity of the liquid detergent, ρ , is defined as the mass per unit volume. The measurement of the specific gravity of the liquid detergent involved weighting a known volume of test liquid and then calculating the specific gravity by dividing the mass of liquid by the volume of liquid. During this investigation, 100 cm³ volumetric flasks were used to measure precisely 100 cm³ of liquid detergent. An Ohaus Explorer Pro EP214D analytical balance, accurate to four decimal points, supplied by Fisher Scientific UK Ltd., Loughborough, UK, was used to obtain the weight of the 100 cm³ liquid detergents.

The temperature of the liquid detergents in the volumetric flask was maintained at 20 °C during each measurement using a water-bath having refrigeration capability. The weight of the 100 cm³ liquid detergent was measured three times and average taken.

4.3. Procedure for the measurement of surface tension

The surface tension of a liquid is defined as “the force acting over the surface per unit length of surface perpendicular to the force”.

Several methods for the measurement of the surface tension, such as, capillary rise, Wilhelmy plates and drop-weight, are available. During this study, platinum ring method was used. Thus, a du Nouy tensiometer, a surface tension torsion balance supplied by Torsion Balance Supplies, Malvern Wells, Worcestershire, UK, was employed. Five measurements for each liquid sample were carried of which the average was taken as the surface tension of the liquid sample.

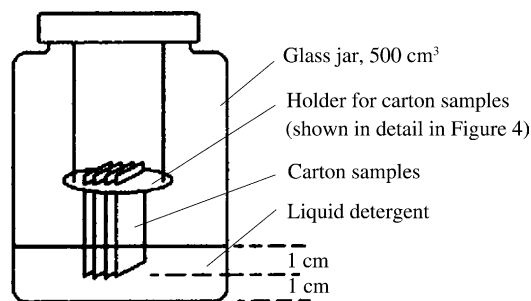


Fig. 3. Schematic illustration of the in-house built device for wicking tests.

4.4. Procedure for the measurement of viscosity

For the determination of viscosity of the liquids, a Brookfield model DV-II+ viscometer (supplied by Brookfield Viscometers Ltd., Harlow, Essex, UK) was used.

4.5. Procedure for the measurement of particle size and size distribution

A COULTER N135 particle size analyser supplied by Beckman Coulter Ltd., High Wycombe, Buckinghamshire, UK was used for the analysis of particle size and size distribution.

4.6. Procedure for the evaluation of the rate of wicking

The rate of wicking of liquid detergent through carton board was determined by measuring the weight gain of the carton board of defined dimension of which one end was in contact with the liquid detergent, over a period of time. An in-house built device, Fig. 3, was used for wicking tests. The holder for the carton samples is shown, in greater details, in Fig. 4.

The open-topped glass jar containing the carton sample and the liquid detergent was placed in an electric oven with temperature control.

Carton board was cut to strips of dimensions 3 cm × 7 cm for wicking tests. For the evaluation of the rate of wicking, both edges along the length of the carton samples were sealed with wax. However, for the investigation of the potential of wicking, un-sealed carton samples were also used.

The temperature of the test cabinet, i.e. the electric oven, was maintained at 25 °C. The humidity of the test cabinet was

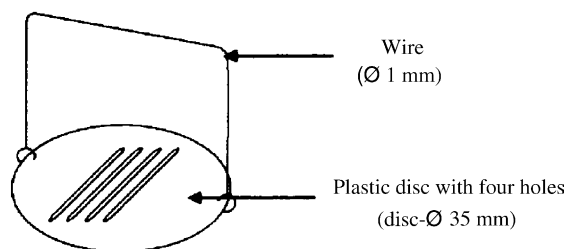


Fig. 4. Schematic illustration of the in-house built holder for carton sample.

Table 1
Physical chemistry properties of the liquid detergents

Liquid detergent	Density, ρ (kg/m ³)	Surface tension, σ (N/m)	Viscosity, μ (Pa s)	Particle size ^a , ϕ ($\times 10^{-6}$ m)
D1	1075	0.0315	0.537	2.1
D2	1023	0.0319	0.265	5.4
D3	1019	0.0333	0.022	2.1
D4	1262	0.027	1.120	3.6
D5	1001	0.037	0.112	7.2
D6	994	0.0329	0.065	35.0

^a Size of 95% of particles.

maintained at 50%, using a total of 1000 cm³ saturated aqueous solution of sodium hydrogen sulphate (1 g/cm³), placed in the cabinet.

The weight of each of the four carton samples was measured and recorded prior to placing into the glass jar. The carton samples were taken out of the glass at an interval of 24 h. The excess liquid detergent was wiped off the carton samples using soft tissues. The carton samples were then weighed before returning to the glass jar for the continuation of the wicking tests.

All six liquid detergents were subjected to wicking test.

5. Results and discussion

5.1. Physical–chemical properties of the liquid detergents

The specific gravity, the surface tension and the viscosity of each of the six liquid detergents investigated are given in Table 1.

It can be seen, from Table 1, that the liquid detergents employed for the investigation reported here had various property attributes, in particular the viscosity and particle size. Such a variation of the property attributes enabled a thorough investigation of the relationship between the wicking behaviour and the properties of the liquid detergents. It should be pointed out that the particles within all the detergents investigated followed similar size distribution profiles. As such, the

particle size distribution characteristic was not included as a parameter of concern in the investigation reported here.

5.2. Wicking behaviours observed

The unsealed carton samples, after 216 h of wicking test, are shown in Fig. 5.

It can be seen from Fig. 5 that both D1 and D2 were aggressive detergents in terms of wicking into the carton packaging material. The order of the extent of wicking appears to be D1 > D2 > D3 > D6 > D4 ~ D5. Comparing such an order of extent of wicking to the physical–chemical properties of the relevant liquid detergents, it can be seen that the particle size and the viscosity of the liquid detergent had a significant effect on the extent of wicking. Thus, D1–D3 having relatively small particles and relatively low viscosities, caused greater extents of wicking.

It can also be seen, from Fig. 5, that liquid detergents tended to wicking through all open edges of the carton samples. This is an indication that wicking through the carton is not significantly dependent on the specific gravity of the liquid detergent.

The appearance of the edge-sealed carton samples, after 9 days of wicking test is shown in Fig. 6.

It can be seen, from Fig. 6, that the liquid detergents now only wicked through the unsealed, bottom edge of the carton samples. It is also clear, from Fig. 6, that D3 behaved differently from other liquid detergents. Thus, D3 appeared to have wicked through the carton at a much higher rate than other liquid detergents. This is likely due to the fact that D3 has a very low viscosity, therefore, a greater mobility through the carton structure.

The weight gains of the sealed carton samples, at various stages during the wicking test, are given in Table 2.

It can be seen, from Table 2, that D3 had the highest rate of wicking. It can also be seen, from Table 2, that the order of the rate of wicking follows: D3 > D1 > D2 > D6 > D5 > D4. Such observations are more reliable than those obtained based on the visual judgement, which did not allow the assessment of the wicking within the carton sample.

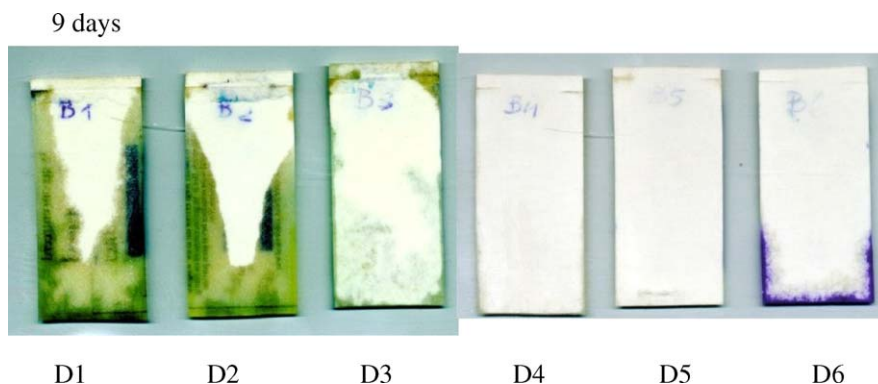


Fig. 5. Appearance of open-edged carton samples after 216 h of wicking test.

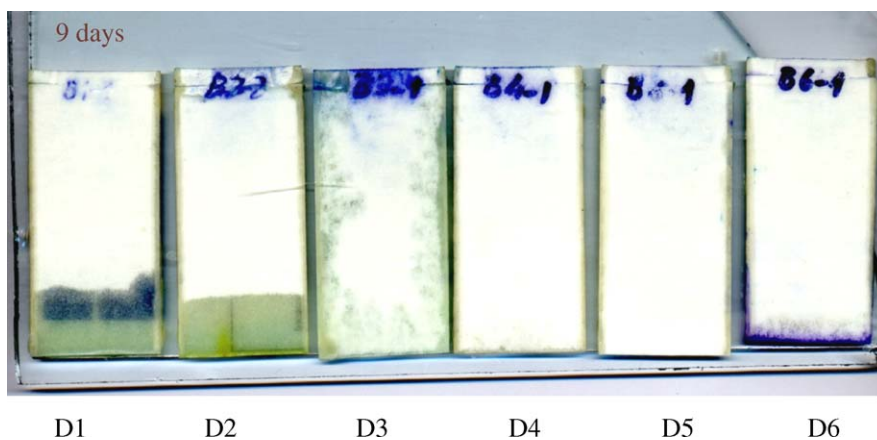


Fig. 6. Appearance of edge-sealed carton samples after 216 h of wicking tests.

Table 2

Weight gains of edge-sealed carton samples after wicking

Time of wicking (h)	Weight gains after wicking tests, W (g)					
	D1	D2	D3	D4	D5	D6
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
18	0.0789	0.0486	0.1794	0.0188	0.0188	0.0331
23	0.0818	0.0518	0.2045	0.0230	0.0224	0.0347
48	0.1052	0.069	0.2768	0.0295	0.0403	0.0594
72	0.1221	0.0791	0.305	0.0383	0.0568	0.0744
96	0.1363	0.0993	0.3335	0.0453	0.0662	0.0894
168	0.1519	0.1158	0.3694	0.0576	0.0833	0.1373
192	0.1691	0.1283	0.3912	0.0639	0.0895	0.1492
216	0.1790	0.1378	0.4154	0.0689	0.0982	0.1597
240	0.1853	0.1461	0.4307	0.0761	0.1039	0.1674
264	0.1940	0.1547	0.4420	0.0801	0.1089	0.1769

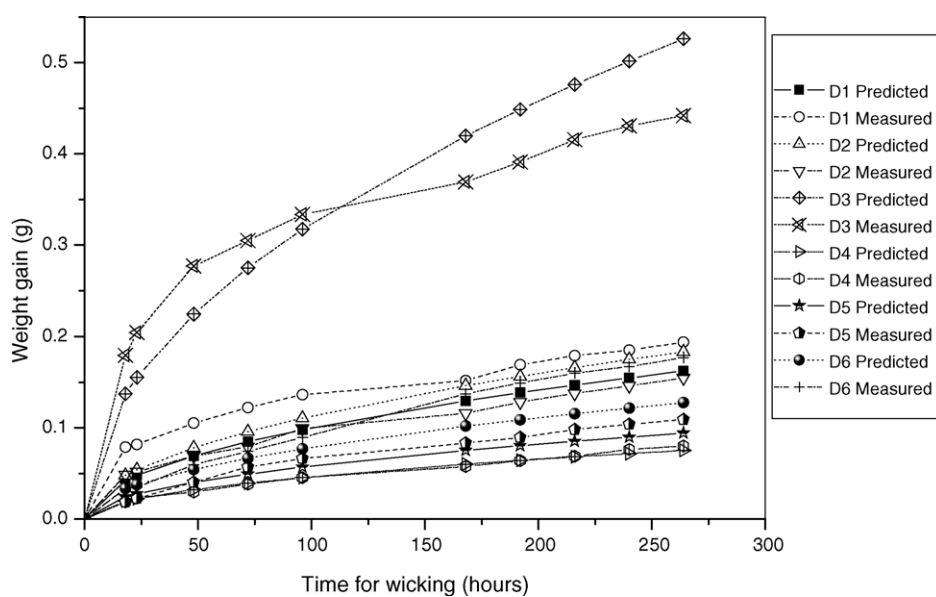


Fig. 7. Comparison of the predicted and measured profiles of weight gains on carton sample.

5.3. Modelling of the wicking

An attempt was made to obtain the coefficients c_1 – c_5 for wicking model, Eq. (5), using the data obtained. The MAPLE software (supplied by Maplesoft, 615 Kumpf Drive, Waterloo, Ont., Canada) was used for obtaining the coefficients. The linear regression function within the MAPLE V software was used for such a purpose. Thus, Eq. (5) was converted into Eq. (6):

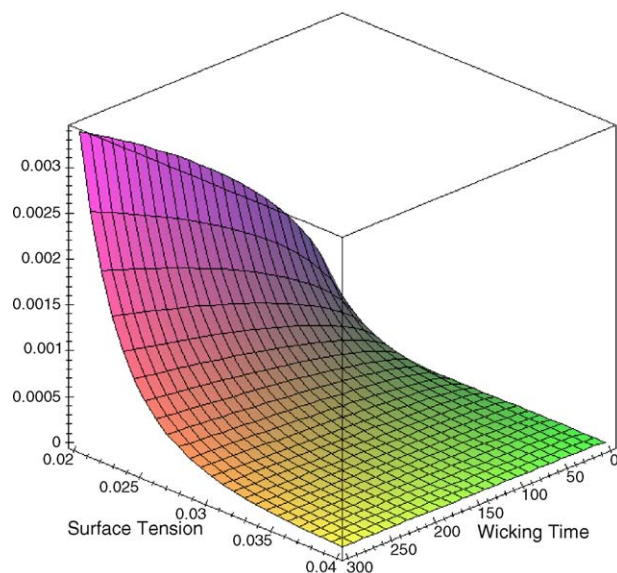
$$\ln(W) = \ln(c_1) + c_2 \ln(\sigma) + c_3 \ln(\phi) + c_4 \ln(\mu) + c_5 \ln(\rho) + \frac{1}{2} \ln(t) \quad (6)$$

Let $C_1 = \ln(c_1)$ and rearrange Eq. (6), we have Eq. (7):

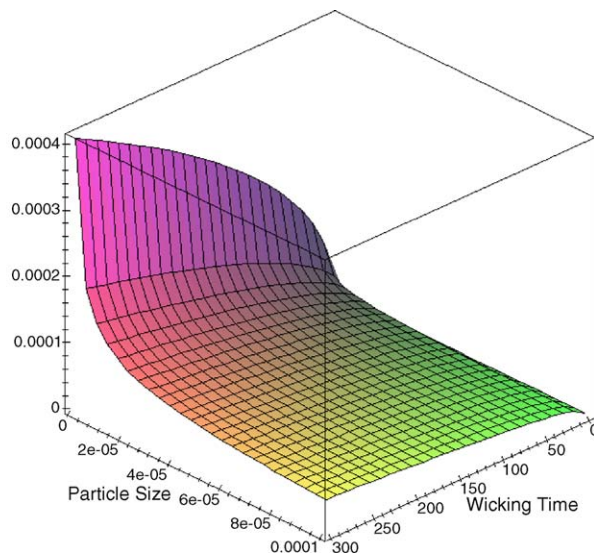
$$C_1 + c_2 \ln(\sigma) + c_3 \ln(\phi) + c_4 \ln(\mu) + c_5 \ln(\rho) = \ln(W) - \frac{1}{2} \ln(t) \quad (7)$$

Using the data given in Tables 1 and 2, a series of equations were created based on Eq. (7). For instance, using the data relevant to the weight gain of the carton after wicking with detergent D1 ($\sigma = 0.0315$ N/m; $\phi = 0.0021$ m; $\mu = 0.537$ Pa s; $\rho = 1075$ kg/m³) for 18 h ($t = 64\,800$ s and $W = 7.89 \times 10^5$ kg), Eq. (8) can be created:

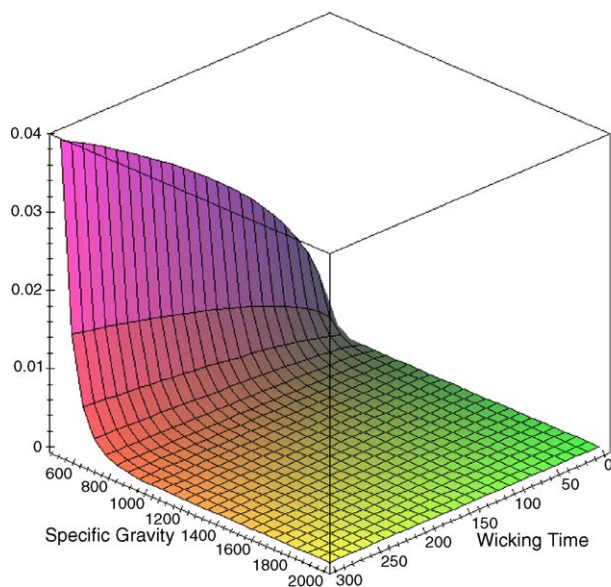
$$C_1 - 3.46c_2 - 6.17c_3 - 0.62c_4 + 6.98c_5 = -14.99 \quad (8)$$



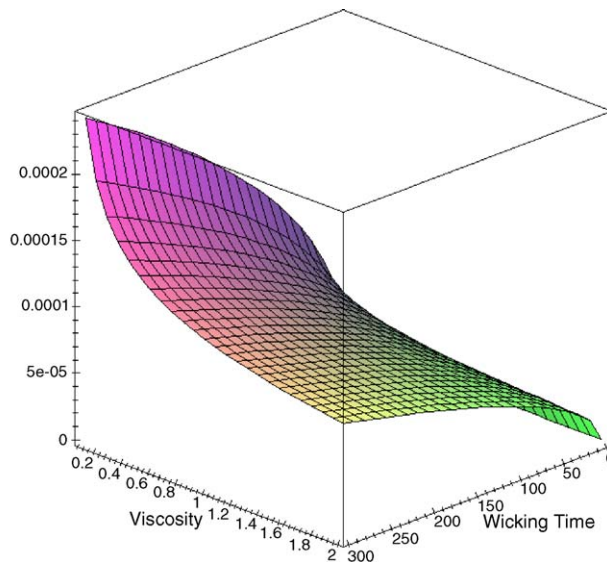
Weight gain vs. Surface tension and Time



Weight gain vs. Particle size and Time



Weight gain vs. Specific gravity and Time



Weight gain vs. Viscosity and Time

Fig. 8. The dependence of weight gain on various physical–chemical properties of the liquid detergent.

Based on the weight gain data for six detergents, a total of 60 equations similar to Eq. (8) (10 weight gains were obtained each at 18, 23, 48, 72, 96, 168, 192, 216, 240 and 264 h for each detergent, respectively) were obtained.

Using the “Leastsqrs” function within the MAPLE software package, the best fit coefficients c_1 – c_5 were obtained. These were

$$c_1 = 8.67 \times 10^4, \quad c_2 = -6.81, \quad c_3 = -0.47, \\ c_4 = -0.35, \quad c_5 = -8.15$$

Thus, the relationship between the weight gain of the carton board sample and the surface tension, the mean particle size, the viscosity and the density of the liquid detergent could be expressed by Eq. (9):

$$W = \frac{8.67 \times 10^4 t^{1/2}}{\sigma^{6.81} \phi^{0.47} \rho^{8.15} \mu^{0.35}} \quad (9)$$

The accuracy of the model of wicking, represented by Eq. (9), was assessed by comparing the predicted weight gains of the carton to the measured values. Thus, the profiles of the predicted weight gains of the carton samples and of the measured ones are shown in Fig. 7.

It can be seen, from Fig. 7, that the model gives relatively accurate predictions of the profiles of weight gain of the carton sample.

5.4. Dependence of the rate of wicking on properties of the liquid detergent

Based on the model of wicking, Eq. (9), it was then possible to visualise the dependence of the rate of wicking on the properties of the liquid detergents. Relevant three-dimensional graphs, based on Eq. (9), are shown in Fig. 8.

It can be seen, from Fig. 8, that the weight gain of the carton sample is more significantly dependent on the particle size and the viscosity of the liquid detergent. At the wicking progresses, the effects of particle size and viscosity of the liquid detergent on the rate of wicking increases.

6. Conclusions

It can be concluded that the rate of wicking of liquid detergent through carton packaging is dependent on the physical–chemical properties of the liquid detergent such as the particle size characteristics, the viscosity, the specific gravity and the surface tension. Among various physical–chemical properties, the particle size characteristics and the viscosity had more significant effects on the rate of wicking. Thus, liquid detergents having larger particles and a higher viscosity would have a lower rate of wicking through carton packaging.

Based on the experimental data obtained through the investigation reported here, a mathematical model for the simulation of the relationship between the weight gain of the carton, due to wicking of the liquid detergent, and the physical–chemical properties of the liquid detergent namely, mean particle size, viscosity, specific gravity and surface tension was obtained. Such a model gave relatively accurate prediction of the weight gain of carton due to wicking for detergents of various physical–chemical properties. Such a model could be used by packaging industry for the selection of carton packaging materials, based on the readily obtainable physical–chemical properties of the liquid detergent.

The principal associated with the construction of mathematical model for wicking of liquid detergent through carton packaging, developed through the investigation reported here, could be used for future development of models for wicking or diffusion through packaging materials.

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