

MODELLING OF THE DRYING PROCESS OF POLYURETHANE FOAM

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Abstract—The drying process of a polyurethane (PU) sheet is studied with the help of experiments and a numerical model, by considering not only the evaporation of the liquid water but also the diffusion of the vapour through the foam. Because of this evaporation, the front of the liquid in contact with the vapour is assumed to move through the foam. There is thus a problem with moving boundaries. The rate of evaporation is proportional to the gradient of the vapour concentration at the liquid front and also to the rate of motion of this front. In spite of the fact that a concentration-dependent diffusivity can be accounted for by the model, the diffusivity of the vapour is assumed to be constant throughout the process. The rate of vapour release out of the external surface of the PU sheet is proportional to the difference between the actual concentration of vapour at the PU surface and the concentration required to maintain equilibrium with the surrounding atmosphere, and also to the gradient of concentration of vapour at this surface. The model is able to provide kinetics of drying correlating well with experiments, with a constant rate of drying during a large part of the process.

INTRODUCTION

Because of their mechanical properties, such as flexibility and ability to absorb shocks as well as their good weather-resisting characteristics, polyurethane (PU) foams are widely used, especially in cars and buildings. Other properties are also of interest, such as very low heat conductivity, and PU foam sheets are capable of reducing heat transfer. In many of these applications, the PU foam may be in contact with other materials: (i) plasticized PVC [1], or (ii) a liquid, and the plasticizer or the liquid generally diffuse into the foam to the detriment of its properties. The complementary problem is the ability of the PU foam to dry after its extraction from the liquid.

The first purpose in this paper is to study the process of desorption of a liquid out of a PU foam sheet which has been previously presaturated. The liquid selected is water, and two temperatures, 100° and 80°, are chosen, because of the long time of experiment needed at ordinary temperatures. As the sheet is very thin, a 1-dimensional transport can be considered [2, 3], the liquid transport through the edges of the sheet being neglected.

The second objective in this study is to build up a numerical model capable of describing the process, and especially the constant rate of drying during a large part of the process. The process is rather complex, with the vapour–liquid boundary moving within the sheet, and the following facts have to be considered:

- (i) the evaporation of the liquid responsible for the water–vapour interface moving from the external surface to the inside of the sheet;

- (ii) the diffusion of the vapour through the part of the sheet free from liquid water;
- (iii) the elimination of the vapour from the external surface of the sheet.

In spite of the fact that the transport of vapour may take place in response to a pressure gradient [4] and not to a concentration gradient, as shown in pieces of wood, most wood scientists have assumed that the driving force is the gradient of concentration of moisture within the solid [2, 3, 5, 6]. As wood consists essentially of open cells connected in the same way as in PU foam, this assumption of diffusion of vapour through the foam is considered.

THEORETICAL

Assumptions

The following assumptions are made:

- (i) The process of drying is controlled by evaporation of the water, and diffusion of the vapour.
- (ii) The transfer of water is perpendicular to the sheet.
- (iii) The boundary between the liquid and vapour moves from the surface into the inside of the PU sheet, as evaporation proceeds.
- (iv) The temperature is constant during the whole process.
- (v) The rate of vaporization of the water at the liquid–vapour interface is equal to the rate at which the vapour is extracted by diffusion and also is proportional to the rate of motion of this interface.

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- (vi) The diffusivity of the vapour within the foam is constant. The diffusivity of the liquid is assumed to be zero, so that the liquid concentration is constant in the liquid phase.
- (vii) The rate of release of vapour out of the PU surface is proportional to the gradient of vapour concentration at this surface, and to the difference between the actual concentration on the surface and the concentration required to maintain equilibrium with the surrounding atmosphere.
- (viii) The pressure within the PU sheet does not change during the process.
- (ix) The change in dimensions of the sheet is neglected.

Mathematical treatment

The following basic equations are used to describe the process.

The first equation expresses the ratio of the concentration of vapour and liquid on each side of the front of vaporization (abscissa X_i).

$$C_v(X_i, t) = r \cdot C_L(X_i, t) \quad (1)$$

where r is the ratio between the densities of vapour and liquid at the temperature considered. Here $C_L(X_i, t)$ is assumed constant, equal to C_L .

The second equation represents the rate of vaporization at the beginning of the process, when the front of liquid water is on the PU surface:

$$F_0 = \frac{dX_i}{dt} [C_L(0,0) - C_v(0,0)]. \quad (2)$$

The matter balance through the liquid-vapour interface at position X_i and time t is written thus:

$$D_v \cdot \frac{\partial C_v}{\partial x}(X_i^-, t) = \frac{dX_i}{dt} [C_L(X_i^+, t) - C_v(X_i^-, t)]. \quad (3)$$

The diffusion of the vapour from the water front to the external surface of the PU is expressed by:

$$\frac{\partial C_v}{\partial t} = C_v \cdot \frac{\partial^2 C_v}{\partial x^2} \quad \text{with } 0 < x < X_i \quad (4)$$

when the diffusivity is constant.

The rate of elimination of the vapour out of the PU surface is equal to the rate at which the vapour is brought to the PU surface by internal diffusion, and is also proportional to the effective concentration of vapour at the surface (abscissa zero):

$$F_i = F_0 \cdot \frac{C_v(0, t) - C_v(\text{ext}, t)}{C_v(0, 0) - C_v(\text{ext}, 0)} = D_v \cdot \frac{\partial C_v}{\partial x}(0, t). \quad (5)$$

The concentration $C_v(0, 0)$ is given by equation (1),

$$C_v(0, 0) = r \cdot C_L$$

where C_L is the initial concentration of liquid water in the sheet.

$C_v(\text{ext}, t)$ is the internal concentration of vapour required to maintain equilibrium with the surrounding atmosphere. The volume of this atmosphere is very large so that the concentration of vapour is close to zero

$$C_v(\text{ext}, t) = 0.$$

Equation (5) thus becomes:

$$F_i = K \cdot C_v(0, t) = D_v \cdot \frac{\partial C_v}{\partial x}(0, t) \quad (5')$$

with

$$K = \frac{F_0}{r \cdot C_L}.$$

Numerical analysis

No analytical solution can be obtained for the problem, and a numerical model with finite differences is built. The thickness of the sheet is divided in $2N$ equal parts of thickness Δx . Let j_t be the integer of $X_i/\Delta x$. The process is studied at various positions:

Within the PU sheet at the liquid-vapour interface. If $j_t \geq 2$, a parabolic approximation is used for the gradient in the left-hand member of equations (3):

$$\begin{aligned} \frac{\partial C_v}{\partial x}(X_i^-, t) &= \frac{3C_v(j_t, t) - 4C_v(j_t - 1, t) + C_v(j_t - 2, t)}{2 \cdot \Delta x}. \end{aligned} \quad (6)$$

Equation (3) becomes:

$$\begin{aligned} D_v \frac{3C_v(j_t, t) - 4C_v(j_t - 1, t) + C_v(j_t - 2, t)}{2 \cdot \Delta x} &= \frac{\Delta X_i}{\Delta t} [C_L - r \cdot C_L] \end{aligned} \quad (7)$$

ΔX_i can thus be calculated from equation (7).

If $j_t = 1$, as the parabolic approximation of the gradient cannot be used, equation (7) is written thus:

$$D_v \cdot \frac{C_v(1, t) - C_v(0, t)}{\Delta x} = \frac{\Delta X_i}{\Delta t} [C_L - r \cdot C_L]. \quad (8)$$

If $j_t = 0$, the left-hand member is replaced by the flux leaving the sheet:

$$K \cdot C(0) \cdot \Delta t - \Delta X_i \cdot (C_L - r \cdot C_L). \quad (9)$$

For obtaining the new concentration $C_N(j_t)$ at time $t + \Delta t$, we write the gradient in two ways, if $j_t \geq 1$:

$$\frac{r \cdot C_L - C_N(j_t)}{X_i - j_t \cdot \Delta x} = \frac{C(j_t) - C(j_t - 1)}{\Delta x}. \quad (10)$$

Before if $C(j_t) = C_L$ we must put $C(j_t) = r \cdot C_L$, because it is the first time that X_i exceed $j_t \cdot \Delta x$.

Release of vapour at the PU surface ($x = 0$). When $j_t \geq 2$, parabolic approximation for the gradient can be used in equation (5') which becomes:

$$K \cdot C_v(0, t) = D_v \frac{4C_v(1, t) - 3C_v(0, t) - C_v(2, t)}{2 \cdot \Delta x} \quad (11)$$

or

$$C_v(0, t) = D_v \frac{4C_v(1, t) - C_v(2, t)}{2K \cdot \Delta x + 3 \cdot D_v}. \quad (12)$$

For $j_t = 1$, the gradient at abscissa 0 is approximated by the gradient at the position $\frac{1}{2}$ and the concentration is thus given by:

$$C_v(0, t) = \frac{D_v \cdot C_v(1, t)}{K \cdot \Delta x + D_v}. \quad (13)$$

For $j_t = 0$, we write:

$$r \cdot C_L - C(0) = \frac{\partial C}{\partial x} \cdot X_t = \frac{K \cdot C(0)}{D_v} \cdot X_t \quad (14)$$

hence

$$C(0) = \frac{r \cdot C_L}{1 + X_t \cdot K/D_v} \quad (15)$$

Diffusion of the vapour within the PU sheet. Equation (4) expressing the diffusion of vapour with constant diffusivity is used for evaluating the vapour balance within the slice of thickness Δx located between the positions $(i - \frac{1}{2})$ and $(i + \frac{1}{2})$. The new concentration after elapse of time Δt at position i is thus obtained as a function of the previous concentration at this place and adjacent places $(i - 1)$ and $(i + 1)$.

$$CN_v(i, t) = \frac{1}{M} [C_v(i + 1, t) + (M - 2) \cdot C_v(i, t) + C_v(i - 1, t)] \quad (16)$$

for $1 \leq i \leq j_t - 1$ if $j_t < N$, or for $1 \leq i \leq N$.

with the dimensionless number M :

$$M = \frac{(\Delta x)^2}{D_v \cdot \Delta t}$$

Symmetry. We use the symmetry by putting:

$$C(N + 1) = C(N - 1).$$

Amount of water in the sheet

The amount of liquid water is

$$ML = C_L \cdot (L - 2X_t) \cdot S$$

where L is the thickness of the sheet and S is its area.

The amount of water in the vapour state is:

if $j_t \geq 3$

$$M_v = \left[\frac{3}{8}(C(0) + C(j_t)) + \frac{9}{8}(C(1) + C(j_t - 1)) + \sum_{j=2}^{j_t-2} C(j) + \frac{1}{2}(C(j_t) + r \cdot C_L) \right] \times \left(\frac{X_t}{\Delta x} - j_t \right) \cdot 2S \cdot \Delta x$$

if $j_t = 2$

$$M_v = \left[\frac{1}{3}(C(0) + C(2)) + \frac{4}{3}C(1) + \frac{1}{2}(C(2) + r \cdot C_L) \right] \times \left(\frac{X_t}{\Delta x} - 2 \right) \cdot S \cdot \Delta x \cdot 2$$

if $j_t = 1$

$$M_v = \left[\frac{1}{2}(C(0) + C(1)) + \frac{1}{2}(C(1) + r \cdot C_L) \right] \times \left(\frac{X_t}{\Delta x} - 1 \right) \cdot S \cdot \Delta x \cdot 2$$

if $j_t = 0$

$$M_v = (C(0) + r \cdot C_L) \cdot X_t \cdot S.$$

Table 1. Rate of evaporation and diffusivity of vapour

Temperature (°C)	Rate of evaporation (g/cm ² /sec)	Diffusivity (cm ² /sec)
80	5×10^{-5}	7.5×10^{-3}
100	5.5×10^{-5}	8×10^{-3}

EXPERIMENTAL PROCEDURES

Material

Rectangular samples of 2×2 cm are cut from commercial sheets of PU foams of thickness 0.2 cm and density 0.51 g/cm³. The lateral surface of the sample is covered with a flexible silicone film in order to protect these surfaces from contact with water. A 1-dimensional transfer of water is thus obtained across the thickness of the sheet.

Experiments

The PU samples are previously immersed in boiling water, or in water at 80°. The kinetics of absorption are followed by weighing the samples at intervals. The pre-saturated samples are thus let free in the surrounding air either at 100° or at 80°. The kinetics of desorption are obtained by weighing the samples at intervals.

RESULTS

Testing the validity of the model is the main point of interest, by using data obtained from experiments: diffusivity of vapour, rate of evaporation of the water. Further insight into the nature of the process is afforded by calculating some profiles of concentration developed through the thickness of the PU sheet.

Determination of the parameters

The rate of evaporation of the water out of the PU sheet is determined from the experimental kinetics of desorption, taken at the beginning of the process. The diffusivity for the water vapour transport is obtained by comparing the experimental kinetics of desorption with the calculated kinetics, and by selecting the value which fits best. The values of the rate of evaporation of the water and of the diffusivities are given in Table 1.

Validity of the model

The validity of the model is tested by comparing the kinetics of desorption obtained either by experiment or by calculation. We have taken $N = 40$. Figure 1 represents the kinetics of desorption at 100°

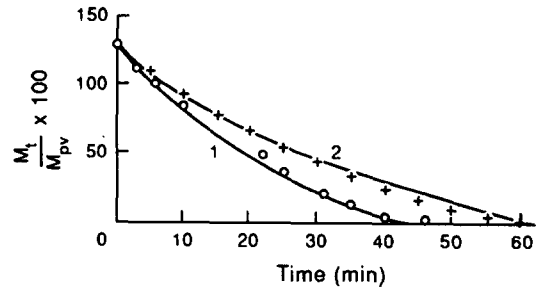


Fig. 1. Kinetics of drying of a PU foam, at 100°C (O) and 80°C (+). —, calculated; O, +, experiments.

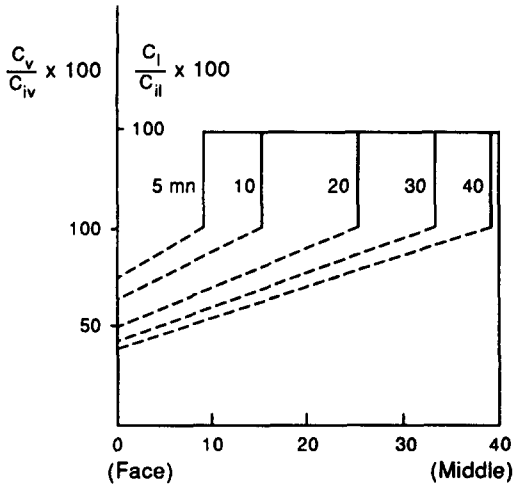


Fig. 2. Profiles of concentration developed through the thickness of the PU foam, at various times, at 100°C (—, liquid water; ---, vapour water). Two scales are given: C_v for vapour, and C_l for liquid water.

and 80°C resulting from experiment and calculation. The following conclusions can be drawn:

- (i) Good agreement is observed between the experimental and calculated kinetics of drying at each temperature.
- (ii) The process is well accounted for by the model, with evaporation of water at constant rate, diffusion of vapour and moving boundary.
- (iii) The rate of drying decreases rather slowly from the beginning to the end of the process.
- (iv) Of course, the rate of drying depends on temperature; obviously the higher the temperature, the faster is the drying.

Profiles of concentration developed through the thickness

The profiles of concentration obtained by calculation with the model are drawn at the two

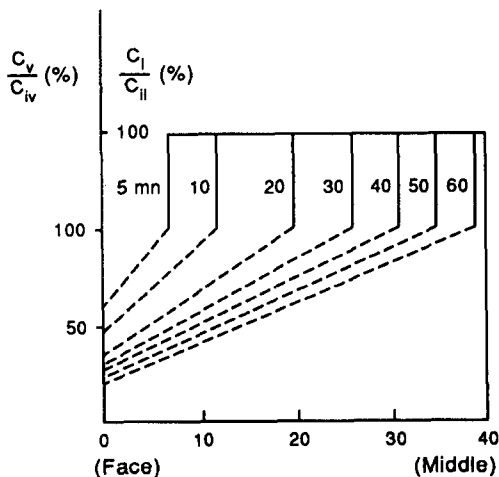


Fig. 3. Profiles of concentration developed through the thickness of the PU foam, at various times, at 80°C (—, liquid water; ---, vapour water).

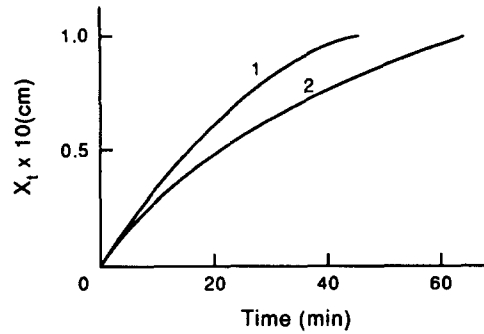


Fig. 4. Displacement of the liquid front with time: 1, 100°C; 2, 80°C.

temperatures: 100°C (Fig. 2) and 80°C (Fig. 3), by considering half the PU sheet located between the external surface and the middle. Some facts are worth noting:

- (i) The evaporating surface of the liquid water moves from the external surface to the middle of the PU sheet.
- (ii) The rate of motion of this evaporating surface decreases regularly from the beginning of the process to the end.
- (iii) Two scales are used for the concentrations of liquid and vapour, as the concentration of the liquid is much higher than that of the vapour from the evaporating surface to the external surface of the PU decreases with a constant rate.
- (iv) The concentration of vapour at the external surface decreases regularly with time.

Rate of displacement of the liquid front

The rate of displacement of the liquid front during the desorption is obtained by fitting the calculated results with the experiments. The variation of the abscissa of the liquid front as a function of time is shown in Fig. 4, for 80 and 100°C. The following conclusions can be drawn:

- (i) Of course the rate of the progressing front of liquid in PU foam is higher at 100°C than at 80°C.
- (ii) Simple mathematical expressions are found for these curves:

$$100^\circ X_l = 0.0055 \cdot (t)^{0.7925} \quad \text{for } t < 43 \text{ min}$$

$$80^\circ X_l = 0.0053 \cdot (t)^{0.7234} \quad \text{for } t < 62 \text{ min.}$$

These expressions are nearly the same, with a higher value for the coefficient at 100°C (2.4 instead of 1.8).

CONCLUSIONS

This paper is devoted to the drying process of a sheet made of a PU foam. The problem is rather complex, in the sense that the kinetics of drying do not follow the usual shape obtained with various polymers (6).

A model based on a numerical method with finite differences is built in order to describe the process. The following assumptions are made:

- (i) The front of the surface of liquid is displaced during the process from the PU surface to the middle of the foam. The rate of displacement as obtained, decreases regularly with time.
- (ii) The vapour diffuses through the channels of the PU foam with a constant diffusivity.

Of course these two transports take place simultaneously but in different places through the PU foam.

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