



Study of the Profile Concentration of a Chemical Through a Sandwich Packaging

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ABSTRACT

The process of chemical transfer is studied through a sandwich packaging, we have been determined the profile of concentration of a chemical through a sandwich packaging in order to understand this phenomenon. The method used for determining the profile of concentration of the chemical in the polymer, based on numerical analysis, given in two parts: The first part is done by putting in contact two polymer sheets, one containing the chemical while the other is free from this chemical. The diffusivity when the chemical leave the first sheet is same when this chemical enters inside the other sheet. The second part is done by putting the sheet of the polymer containing the chemical in contact with two virgin sheets. The diffusivity when the chemical leave the first sheet is same when this chemical enters inside two other sheets.

Key words: Sandwich packaging, Plastic, Modeling, Finite D.M, Diffusion.

INTRODUCTION

Polymer Materials take a good place in the packaging field⁴, so their contact with some product two types of matter transfer occur⁴. First type when the liquid entering the polymer while the second one same additive or chemicals leave the polymer. Both these transfers are governed by transient diffusion.

The purpose of this study is applied a methods which consists of developing the concentration profile developed through the polymer at various time, this method using to determine the kinetics of change in weight.

Both cases were investigated

When two sheets are in contact, one containing the chemical while the other is free from this chemical

Making two sheets in contact with another sheet containing the chemical.

The second objective of this study is to build a numerical model able to resolve the problem.

MATERIALS AND METHODS

Assumptions

Some assumptions are made so as to simplify this phenomenon⁴⁻⁶.

- In the case of the two sheet system, one sheet is free from chemical, while other contains a chemical.
- In the case of the three sheet system, the sheet containing the chemical located between two virgin sheets.
- The concentration initially is uniform
- The transfer is perpendicular to the face of sheet
- The matter transfer is governed by transient diffusion
- No evaporation of the chemical.

Mathematical treatment

The general equation of one-directional diffusion with constant diffusivity is³

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

With the following initial conditions:

$t=0$ Sheet with chemical $C = C_{in}$

Sheet free from chemical $C = 0$

And $t > 0$ external surfaces $\frac{\partial C}{\partial x} = 0$

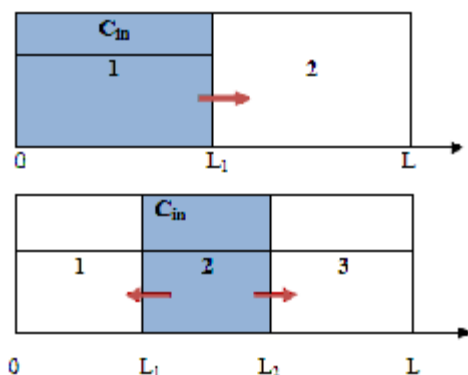


Fig. 1: Scheme of the two and three sheets systems

At the interface between the two polymers sheets, we have [2]:

$$\left| D_1 \frac{\partial C}{\partial x} \right| = \left| D_2 \frac{\partial C}{\partial x} \right| \quad \dots(1)$$

That is mean the rate of liquid transfer is the same on each face of the interface.

The partition factor is the ratio of the concentrations of liquid on each face of the interface:

$$K = \frac{C_2}{C_1} \quad \dots(2)$$

At the interface Analytical solutions

Firstly, it should be noted that the diffusivity is the same in two sheets.

Case of two sheet systems

The profile of concentration of chemical developed through the two sheet systems is given by [3]:

$$\frac{C(x,t)}{C_{in}} = \frac{L_1}{L} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n\pi L_1}{L}\right) \cos\left(\frac{n\pi x}{L}\right) \exp\left(-\frac{n^2 \pi^2}{L^2} Dt\right) \dots(3)$$

With:

- L_1 is the thickness of the diaper where the chemical is initially placed.
- L is the total thickness of the two sheets.
- D is the diffusivity of the chemical in the polymer of the two sheets.

Case of three sheet systems

The profile of concentration of chemical developed with three sheets is given by [4]:

$$\frac{C(x,t)}{C_{in}} = \frac{L_2 - L_1}{L} + \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n(L_2 - L_1)}{2L}\right) \cos\left(\frac{n x}{L}\right) \exp\left(-\frac{n^2 \pi^2}{L^2} Dt\right) \dots(4)$$

with

- $(L_2 - L_1)$ is the thickness of the sheet where the chemical is initially placed.
- L is the total thickness of the two sheets.
- L_1 and $(L - L_2)$ are the thickness of each virgin polymer sheet.
- D is the diffusivity of the chemical in the polymer of the three sheets.

Numerical solution

For all cases, whether an analytical solution exists or not, the numerical treatment is feasible.

We used a Finite difference method (FDM) solution in order to resolve the problem numerically; the principle of this method is to let the range in x be divided into N equal intervals of " x " and time into M equal intervals of " t ". A random point in space and time (x, t) can be represented, by $(i^{\text{th}}x, j^{\text{th}}t)$, where i and j are integers ($i = 1, 2, \dots, N+1$ and $j = 0, 1, \dots, M$). When the profile of chemical concentration is not initially uniform in the source sheet [2], the numerical treatment is the only feasible method [1, 2].

Experimental procedure

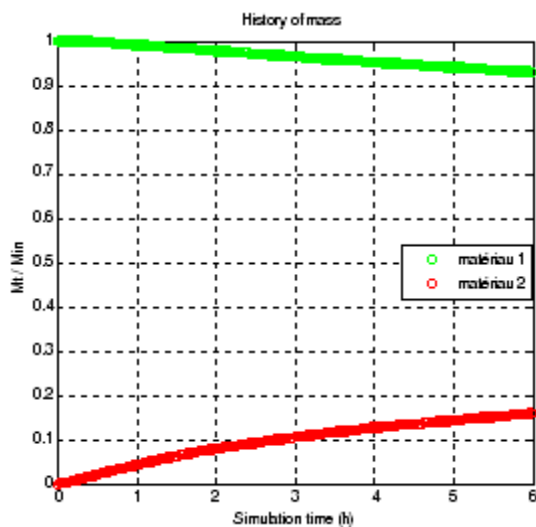


Fig. 2: Evolution of mass in two sheets with simulation time

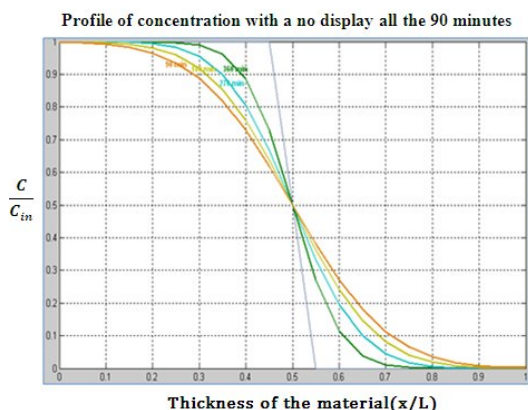


Fig. 3: Profiles of concentration developed through the two sheets system at different times, with the same thickness, ($L_1/L_2=2$) same diffusivity ($D_1/D_2=1$) and $K=1$

We used a scientific software in order to solve the equations for each treatment.

RESULTS AND DISCUSSION

The results are presented in terms of profiles of concentration developed for two and three sheet systems (fig.1) and kinetics diffusion for each system.

For two sheet systems, the chemical is located initially in the sheet on the left. Dimensionless numbers are used so as to make the results general.

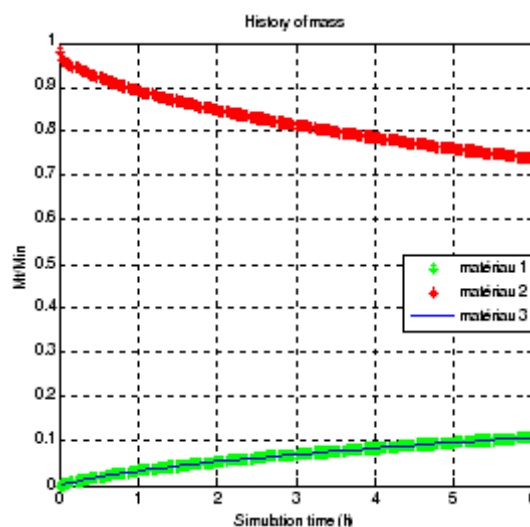


Fig. 4: Evolution of mass in three sheets with simulation time

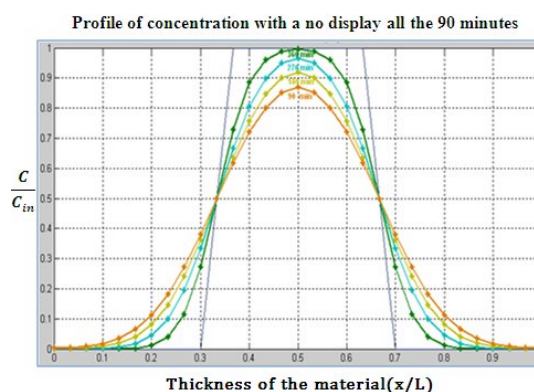


Fig. 5: Profiles of concentration developed through the three sheets system at different times ($D \cdot \Delta t / L^2$), with the same thicknesses, the same diffusivities ($D_1 = D_2 = D_3$) and $K=1$

The coordinates for this contact are: the concentration C at position x and time t as a fraction of the initial concentration C_{in} ; the position x as a fraction of the total thickness L of the sheets system. Dimensionless time is where L is the total thickness of the system.

Figure1. Show us the procedure of contact for two systems (bi-diaper and three diapers).

Figure 2. This figure illustrates the evolution of mass in two sheets as function of simulation time. We observed that when the mass of chemical decrease in the first sheet (containing the chemical) while it increase in the other sheet with same variation.

Figure 3. From this curves that give the profile of concentration developed through two sheets all 90 minutes, we noted that this profile allow to clear the repartition of liquid simulator in these sheets.

Figure4. This figure illustrates the evolution of mass in two sheets as function of simulation time.

We noted that when the mass of chemical decrease in the first sheet (containing the chemical) while it increase in the two other sheets.

Figure 5. Give us the profile of concentration developed through three sheets all 90 minutes. The movement of liquid simulator within the three sheets is clear from this concentration profile.

CONCLUSION

In this article, we studied theoretically two and three sheet systems for determining the profiles of concentration of a chemical developed in these sheets when this chemical was initially placed in one sheet. From the profiles developed we can conclude:

Firstly, these profiles give further information about the nature of the process of the chemical transfer.

Secondly, the diffusivity in a sheet containing the chemical depend the diffusion coefficient in the other sheet virgin.

REFERENCES

1. J. Crank, the Mathematics of Diffusion, Clarendon Press, Oxford, **1975**.
2. J.M. Vergnaud, Liquid Transfer Processes in Polymeric Materials, Prentice Hall Publishers, Englewood Cliffs, NJ, USA, **1991**.
3. J.M. VERGNAUD, «Liquid Transparent Process in Polymeric Materials. Modelling and Industrial Applications», Prentice Hall, Englewood Cliffs, NJ, **1991**.
4. Rachid ATMANI, 2014, «Diffusion of Heptane in Polyethylene Vinyl Acetate: Modelisation and Experimentation», *IOSR Journal of Applied Chemistry (IOSR-JAC)*, **2014** .,7, (6). 82-86.
5. Rachid ATMANI, , «Ethanol Diffusion in Polyethylene Vinyl Acetate: Modelling and Experimentation», *Global Journal of Science Frontier Research Chemistry*, **2013.**, 13 (8).