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ETHANOL DIFFUSION IN POLYETHYLENE VINYL ACETATE MODELLING AND EXPERIMENTATION

Ethanol Diffusion in Polyethylene Vinyl Acetate: Modelling and Experimentation

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I. Introduction

Polymeric materials have become an indispensable part of food packaging. In recent years the plastic takes an important place in food packaging as well as pharmaceuticals and cosmetics packaging.

When a polymer is put in contact with a liquid, some matter transfers may take place. Generally, the process of the liquid transport within the polymer is controlled by transient diffusion. This contact can both contaminate our product and change the mechanical properties of the plastic packaging.

II. Theoretical and Experimental Part

The study the liquid diffusion into a polymer simulator, is based on the following simplifying assumptions:

- The distribution is in accordance with fick's laws.
- The diffusion coefficient is independent of concentration.
- The diffusion in the sphere is three-way.
- The polymer was spherical in shape with a constant radius, as the amount of ethanol is very small.
- The chemical does not evaporate on surface.

a) Analytical processing

When the diffusion is radial, Fick's second law expressing the diffusion equation under transient conditions is in the general form.

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$$\frac{\partial C}{\partial t} = \frac{1}{r^2}.\frac{\partial}{\partial r}\left[D.r^2.\frac{\partial C}{\partial r}\right](eq1)$$

Where C is the concentration at time t and at a distance r from the center of the sphere.

When the diffusivity D is constant, the diffusion equation takes the form of:

$$\frac{\partial C}{\partial t} = D.\left[\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}.\frac{\partial C}{\partial r}\right](eq2)$$

Analytical solutions can be obtained when the diffusivity is constant. Problems with a concentration-dependent diffusivity need numerical methods.

By putting:

$$U = C.r(eq3)$$

Equation (2) becomes:

$$\frac{\partial U}{\partial t} = D.\frac{\partial^2 U}{\partial r^2}(eq4)$$

Equation (4) is similar to the equation obtained for diffusion in one dimension through the plane sheet.

Case study: The initial distribution in the sphere is constant: Ci.

b) Mathematical model

The total amount of diffusing substance going into or leaving the sphere is given by intergrating Fick's first law according to time.

$$M_t = -\int_0^t D.\left(\frac{\partial C}{\partial r}\right)_{r\approx R}.dt(eq5)$$

By considering: $\sum_1^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}$

And: $M_{\infty} = \frac{4}{3}\pi R^3.C_0$

We can obtained:

$$\frac{M_{\infty} - M_t}{M_{\infty}} = \frac{6}{\pi^2}.\sum_1^{\infty}\frac{1}{n^2}.\exp\left(\frac{n^2\pi^2}{R^2}Dt\right)(eq6)$$

Another expression of the solution of the equation of diffusion in the sphere (equation 5) is given by:

$$\frac{C_{r,t}-C_i}{C_0-C_i}=\frac{R}{r}.\sum_0^\infty\left\{erfc\frac{(2n+1)R+r}{2(Dt)^{0.5}}-erfc\frac{(2n+1)R+r}{2(Dt)^{0.5}}\right\}(eq7)$$

The kinetics for the matter transported is:

$$\frac{M_t}{M_\infty}=6\left(\frac{Dt}{R^2}\right)^{0.5}.\left\{\pi^{-0.5}+2\sum_1^\infty ierfc\frac{nR}{(Dt)^{0.5}}\right\}-3\frac{Dt}{R^2}(eq8)$$

Case of short times. Equation (8) is very useful for short times because it can be reduced to:

$$\frac{M_t}{M_\infty}=\frac{6}{R}\left(\frac{Dt}{\pi}\right)^{0.5}\quad(eq9)$$

c) Numerical model - Finite difference method-

Analytical solutions can be obtained when the diffusivity is constant. Problems with a concentration-dependent diffusivity need numerical methods. In this case, the problem must be solved by using the numerical Finite difference method.

Case study: The amount of the remaining ethanol within the sphere.

$$M_t=4\pi\int_0^R r^2.C_{r,t}.dr(eq10)$$

This expression can be rewritten using finite difference method.

$$M_t=4\pi(\Delta r)^3.\left[\frac{C_0}{24}+\sum_1^2 n^2C_n+\frac{9}{8}(n-1)^2C_{n-1}+\frac{3}{8}n^2.C_n\right](eq11)$$

d) Experimental procedure

The material used is polyethylene vinyl acetate (also known as PEVA) is the copolymer of ethylene and vinyl acetate. And our product simulator used is ethanol or ethyl alcohol is an alcohol of the structural formula CH3-CH2-OH. It is a colorless, volatil, flammable and miscible with water in all proportions liquid. Contacting: The contacting sample of polyethylene vinyl acetate is carried out with ethanol at 25°C. During the contact, we measured the specific mass of the sphere each time to study the evolution of the mass sphere.

III. Results and Discussions

The percentage of ethanol mass variation inside our plastic sphere (fig.1) is given by the following equation:

$$\Delta m=\frac{m_t-m_0}{m_0}\times 100(eq12)$$

Effect of The diffusion coefficient is given by this relation:

$$D=\pi\left(\frac{\alpha.R}{6}\right)^2\frac{1}{60^2}(eq13)$$

En cm²/s:

$D = 1{,}390.10^{-6}$cm²/s

Figure 2 shows the variation of the amount of ethanol in the PEVA with time, we note that the ethanol in polyethylene vinyl acetate mass increases with the contact time. Until equilibrium reached.

Figure 3 show the amount of ethanol in the material according to simulation time for each solution (analytical, numerical and experience). We notice from this figure that three solutions gives the same variation in the amount of ethanol absorbed as a function of time. So we concluded that the model is validated.

Figure 4 show the profile of the concentration of ethanol after every 10 min.

a. The ethanol concentration within the sphere is low, however the surfaces.
b. This concentration profile is aimed to give good information on ethanol inside PEVA, ie for each point in our sample we can easily determine its concentration.

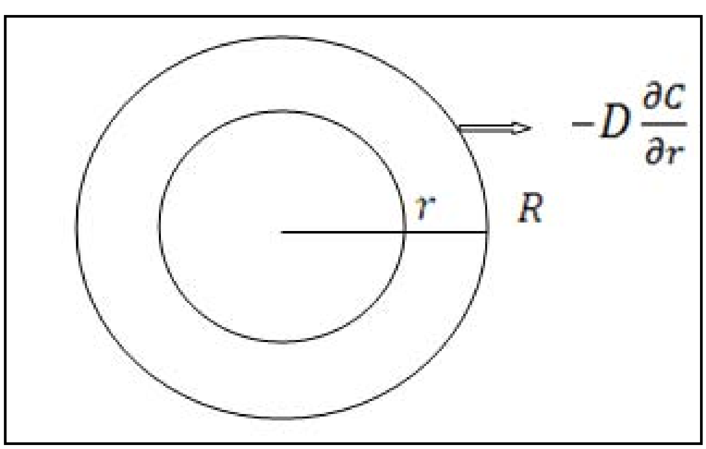

Figure 1 : Schema of the circular cross section of a sphere of radius R.

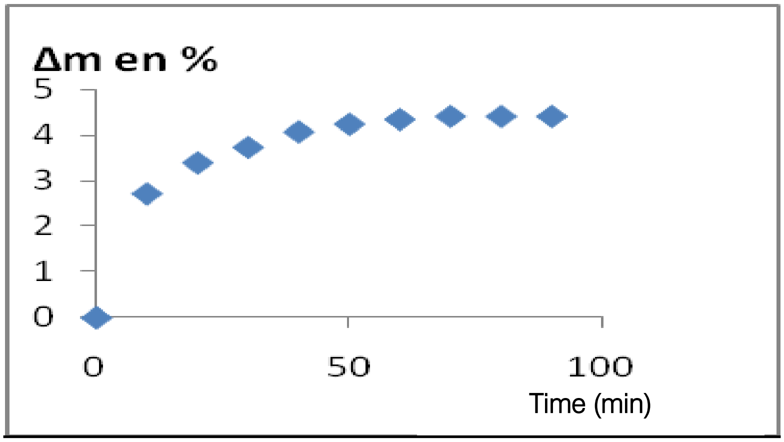

Figure 2 : Variation of the amount of ethanol in the PEVA

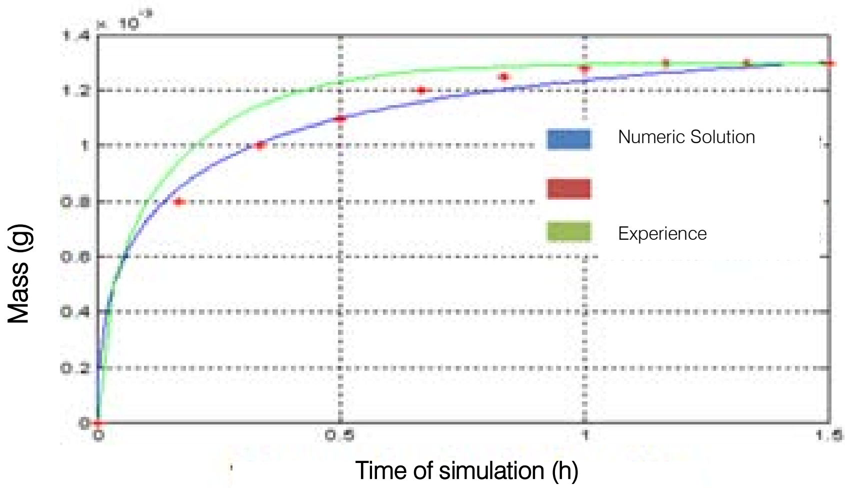

Figure 3 : The amount of ethanol in the material as a function of time for the simulation of three solutions.

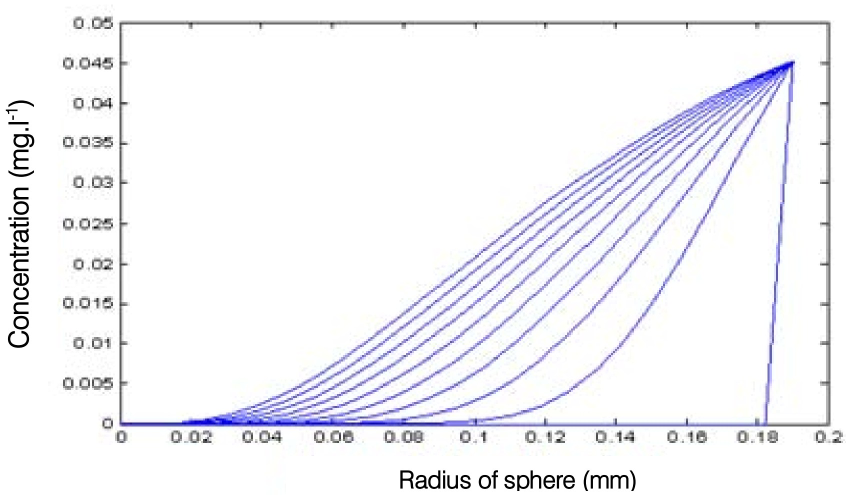

Figure 4 : The profile of the concentration of ethanol after every 10 min

IV. Conclusion

Through this work, we contributed to the study and development of new methods coupling experiments with modeling to understand the behavior of plastic packaging in contact with the food products.

The study was conducted by weighed following the evolution of the mass transferred over time. The polyethylene vinyl acetate contact with ethanol (considered simulating agent) at a temperature of 25◦C, showed that the amount of ethanol in the polymer increases with time.

The resulting profile gives better information on concentrations of ethanol inside the package polyethylene vinyl acetate. In addition, we allow a few hours to simulate mass transfer in reality lasting several months.

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