Polymer Testing 28 (2009) 315–323

Contents lists available at ScienceDirect

Polymer Testing

journal homepage: www.elsevier.com/locate/polytest

Test Method

Non-Fickian diffusion of amyl acetate in polypropylene packaging: Experiments and modelling

Oussama Zaki [a], Boussad Abbès [b,*], Laurent Safa [b]

[a] ENSIB/LEES, Ecole Nationale Supérieure d'Ingénieurs de Bourges, Laboratoire Energétique Explosions Structures, 88 boulevard Lahitolle 18020 Bourges cedex, France

[b] URCA/GRESPI/LMN, Université de Reims Champagne-Ardenne, Groupe de Recherche en Sciences Pour l'Ingénieur (EA 4301), Laboratoire de Modélisation Numérique, Faculté des Sciences, Moulin de la Housse, BP 1039, F51687 Reims cedex 2, France

ARTICLE INFO

Article history:
Received 28 November 2008
Accepted 8 January 2009

Keywords:
Sorption
Non-Fickian diffusion
Polypropylene
Amyl acetate

ABSTRACT

In this paper, we present the methodology and the results obtained by the gravimetric and the FTIR methods to study the sorption of amyl acetate in polypropylene packaging. The influence of the concentration of amyl acetate and the temperature of aging on the sorption is discussed. A non-Fickian model is used to determine the diffusion coefficient and the surface mass transfer coefficient and their evolution with the amyl acetate concentration and the temperature of aging. The effect of the diffusion of amyl acetate on the polypropylene is studied by means of thermal properties.

1. Introduction

Diffusion in polymeric materials is of fundamental importance in many applications and is the subject of considerable scientific interest. The ingress of chemicals into polymers can have a critical effect on the service performance of a component or structure. The diffusion of chemicals in a polymer component may affect the mechanical performance of the material, degrade the material or product that the polymer should protect (e.g. spoiling of packaged foodstuffs, cosmetics or pharmaceuticals), damage the interface between the polymer and another material (e.g. adhesive joints) or pollute the environment.

Diffusion is the concentration gradient driven process whereby the absorbed molecules are transported within the polymer, and diffusion properties are characterised via diffusion coefficients. There is an extensive body of literature on diffusion in plastics and other polymers, e.g. [1–12], reflecting a strong industrial need for reliable test methods to measure the diffusion of gases and liquids in polymers.

In thick sections, such as sheets, pipes and containers, since the time taken to reach equilibrium moisture content is proportional to the square of the thickness, it may take very long periods for equilibrium conditions to be reached. In many applications, the material will see variations in the environment to which it is exposed (e.g. temperature, chemical concentrations) and the mass transport is likely to be a transient problem rather than steady state. It is difficult to test such thick sections reliably since only the early stages of the absorption and permeation curves will be achievable in realistic experimental timescales. Extrapolation of behaviour is necessary to predict long-term behaviour. The options available include: extrapolation of short-term data to long-term behaviour, testing reduced size samples and scaling results to full size through modelling or accelerating mass transport mechanisms through, e.g. higher concentrations or increased temperatures. The study of mass transport in thick sections often involves modelling, requiring good quality data and appropriate models.

There are many measurement methods and several standard techniques for determining mass transport in

* Corresponding author. Fax: +33 3 26913803.
E-mail address: boussad.abbes@univ-reims.fr (B. Abbès).

0142-9418/$ – see front matter
doi:10.1016/j.polymertesting.2009.01.002

polymers such as: nuclear magnetic resonance (NMR) [13,14], laser interferometry [15–17], gravimetric methods [18–27] and Fourier Transform Infra-Red spectroscopy (FTIR) [28–32]. The most suitable method will depend on the type of sample, the diffusing chemical species and the likely rate of diffusion.

The main objective of this work was to study the sorption of amyl acetate in polypropylene packaging using gravimetric and FTIR methods. In addition, the effect of amyl acetate concentration and temperature of aging were evaluated. A non-Fickian model was used to determine the evolution of the diffusion coefficient and the surface mass transfer coefficient. The effect of the sorption of amyl acetate on the thermal properties of polypropylene was also studied.

2. Experimental

2.1. Samples preparation and contact conditions

In this study, we have used samples from commercial extruded blown polypropylene bottles (PP, 0.9–1 mm thick) cut into strips. This polymer is commonly used as a food or cosmetic packaging because of its low weight, flexibility, strength, good moisture barrier and low cost. We had no information about the polypropylene structure and forming conditions. FTIR analysis showed that the polymer is a copolymer polypropylene (CPP) containing 83% of propylene and 17% of methylene monomers.

The amyl acetate (n-pentyl acetate) used is an analytical grade reagent obtained from Aldrich Chemical Company (Lyon, France), with about 99% purity. The product

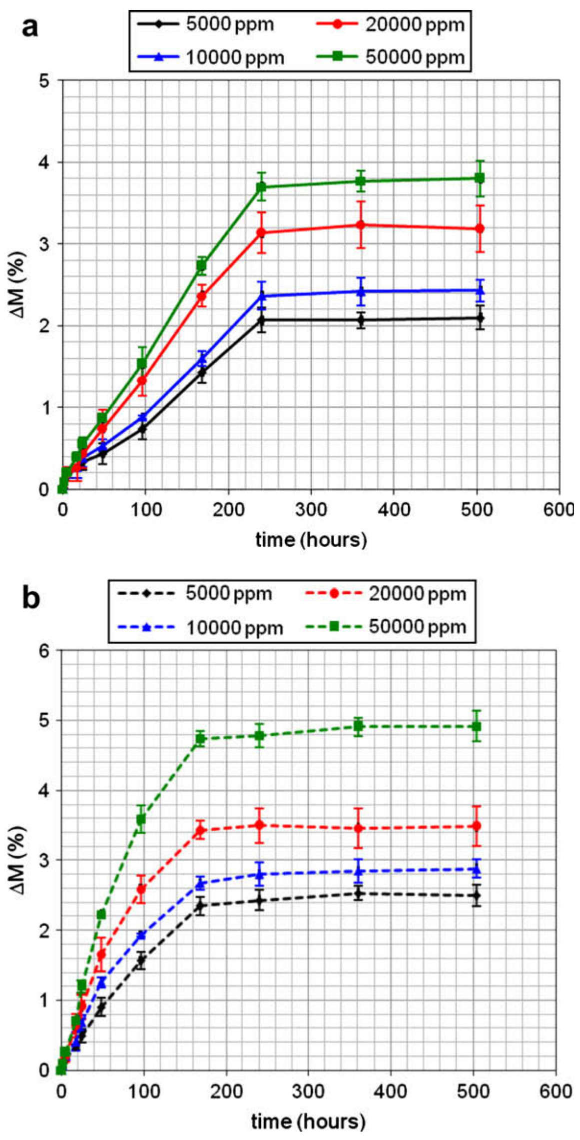

Fig. 1. Relative mass uptake in polypropylene samples for different concentrations of amyl acetate at: (a) 23 °C and (b) 40 °C.

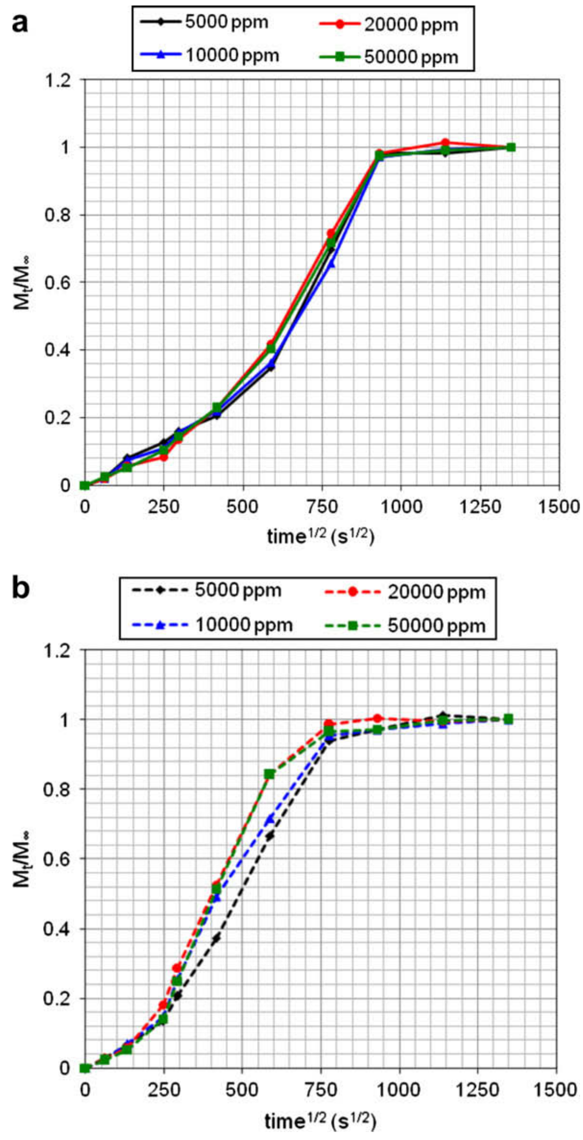

Fig. 2. Gravimetric sorption kinetic curves of amyl acetate into polypropylene samples for different concentrations at: (a) 23 °C and (b) 40 °C.