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Modelling the transport of toluene liquid in protective polymer gloves using a fluorescent dye-tracing technique

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ABSTRACT

The absence of adequate information about the phase change of liquid solvents within polymer-glove walls hinders the complete characterisation of the mass transfer of toluene liquid through the polymer membranes using the data obtained from ASTM F739 method for toluene liquid permeation testing. Therefore, an alternative fluorescent dye-tracing technique is used to account for the transport processes of toluene liquid through polymer gloves. The results of dye penetration experiments show that the displacement of liquid-phase toluene is proportional to the square root of immersion time, indicating that the transport behaviour of liquid-phase toluene is dominated by Fickian diffusion. Furthermore, a linear relationship between the mass sorption of toluene vapour and the sampling time is established, which suggests that the diffusion process in the vapour-phase toluene is governed by Case-II transport. Based on the combined analysis of the results obtained from permeation tests, immersion tests, fluorescent dye-tracer tests, and the pertinent calculations of thermodynamic properties, an evidence-based mechanism for the mass transfer of toluene liquid through the polymer-glove walls is proposed in terms of time-series processes. The model comprises three regimes: a liquid phase, a combined liquid–vapour phase, and a vapour phase of toluene that exist in series within the membrane.

1. Introduction

Protective polymer gloves are widely used in workplaces to reduce the exposure of the workers to hazardous chemicals while handling organic solvents. It is dangerous to use the inappropriate gloves. Thus, an understanding of the chemical-resistance properties of the underlying polymeric materials plays an essential role in making the proper selection of the protective gloves to ensure the safety of the users. Although the transport mechanisms of solvents through polymer materials still remain complex and ambiguous [1,2], it has been known since long that the permeability of the solvents through the polymer membranes depends on two essential properties: solvent solubility and diffusivity [3–5]. In addition, the size and nature of the solvent molecules [6], the composition and structure of the polymer materials [7,8], as well as changes in the polymer structure and mechanical properties due to the solvent-induced effect are important considerations [8–11].

The permeability of the solvents through the polymer gloves is commonly determined using the ASTM F739 standard testing procedure, which characterises the transport properties of organic solvents, such as breakthrough time and permeation rate, and provides an overall decrease in resistance rating. The observed data from the ASTM F739 method can be directly apprehended in terms of a time

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Nomenclature

a_s	activity of toluene liquid
C_0	concentration of toluene liquid (mg cm^{-3})
C_g	concentration of toluene vapour in the collection chamber (μg cm^{-3})
C_s^*	concentration of toluene vapour at liquid–vapour interface (μg cm^{-3})
D_{BR}	diffusion coefficient of toluene liquid in butyl rubber (cm^2 s^{-1})
D_{NR}	diffusion coefficient of toluene liquid in nitrile rubber (cm^2 s^{-1})
E_{va}	evaporation rate of toluene within polymer (mg min^{-1})
F_v	mass flux of toluene vapour (μg min^{-1} cm^{-2})
F_e	equilibrium mass flux of toluene vapour (μg min^{-1} cm^{-2})
k	kinetic constant of Eq. (3)
k_l	kinetic constant of liquid-phase toluene (mg min$^{-0.5}$)
k_v	kinetic constant of vapour-phase toluene (mg min^{-1})
L_0	original membrane thickness (mm)
L_b	membrane thicknesses at breakthrough time (mm)
L_e	membrane thicknesses at steady state (mm)
M	mass sorption of solvent in polymer (mg)
M_L	mass sorption of liquid-phase toluene in polymer (mg)
M_T	total mass sorption of toluene by polymer (mg)
M_V	mass sorption of vapour-phase toluene in polymer (mg)
M_W	molecular weight of toluene (mg)
$\overline{M_c}$	polymer molar mass between crosslinks (g mol^{-1})
n	kinetic exponent of Eq. (3)
P_s^*	equilibrium vapour pressure of solvent at liquid–vapour interface (mmHg)
P_s^{sat}	saturation pressure of toluene solvent (mmHg)
R	universal gas constant (cal/mol K in Eq. (5) or atm-l/mol-K in Eq. (13))
S_d%	saturation swelling ratio of polymer
S_l	solubility of solvent in polymer (g ml^{-1})
Sw_{t_m}	mass-swelling ratio of polymer after a specified immersion time
T	absolute temperature (K)
t	sampling time (min)
t_b	breakthrough time (min)
t_θ	time of the occurrence of liquid–vapour phase coexistence (min)
t_e	time at equilibrium (min)
t_m	immersion time (min)
v	kinetic constant (cm min^{-1})
V_d	volume of dry polymer (ml)
$\overline{V_s}$	molar volume of toluene solvent (cm^3 mol^{-1})
W_{eq}	total mass of the wet polymer at equilibrium (g)
W_d	weight of dry polymer (g)
W_{t_m}	total mass of the wet polymer after a specified immersion time (g)

Greek letters

δ_s	solubility parameter of toluene solvent (cal/cm^3)$^{0.5}$
δ_p	solubility parameter of polymer (cal/cm^3)$^{0.5}$
ϕ_P	polymer volume fraction
ϕ_{pe}	polymer volume fraction at equilibrium
ϕ_S	solvent volume fraction
ρ_p	density of polymer (g ml^{-1})
ρ_s	density of toluene liquid (g ml^{-1})
Φ	penetration depth of toluene liquid (mm)
Φ_{BR}	penetration depth of toluene liquid in butyl rubber (mm)
Φ_{NR}	penetration depth of toluene liquid in nitrile rubber (mm)
χ	polymer–solvent interaction parameter

Mathematical

$\frac{d\Phi}{dt_m^{0.5}}$	derivative of Φ with respect to $t_m^{0.5}$
ΔC	concentration difference between C_s^* and C_g (μg cm^{-3})

record of outlet solvent concentration from the collection chamber of a permeation test cell, represented as a concentration-versus-time (C–t) curve. Meanwhile, a corresponding mass flux-versus-time (F–t) curve can also be derived from a C–t curve based on penetrant mass balance around the permeation test cell [8]. Both the C–t and the F–t curves have characteristic sigmoid shapes indicating a delayed response of solvent breakthrough in the membranes. Many researchers, who have conducted permeability tests for liquid- or vapour-solvent transport in the polymer gloves, have usually used both the C–t and the F–t curves to characterise the mass transfer behaviour of solvents through the polymer membranes [5,8,9,12–15]. However, irrespective of the phase of the solvent feed, notably the outlet solvent in the collection chamber of the permeation test cell is always in the vapour state in the ASTM F739 test. This raises an interesting question of whether the evaporation of the fed liquid solvent occurs on the outer surface of the membrane or within the bulk polymer matrix of the membrane during the permeation process.

According to the studies on liquid–vapour phase transition phenomena for a single liquid compound permeating a membrane [16,17], liquid and vapour solvent phases coexist in the polymer matrices during the liquid penetration process because of the Kelvin effect [18]. In addition, if the feed solvent is a liquid, some of it may be readily converted to the vapour phase inside the polymer matrix during the permeation test because of its high volatility. Moreover, recent studies on solvent vapour transport through the polymer-glove walls [8] indicated that the solvent mass uptake by polymers could be estimated using an F–t curve, in which the estimated amount of mass sorption