



# Simulation analysis of drying of ternary polymeric solution coatings



Raj Kumar Arya<sup>a,\*</sup>, Chitresh Kumar Bhargava<sup>b</sup>

<sup>a</sup> Department of Chemical Engineering, Thapar University Patiala, Bhadson Road, Patiala 147004, Punjab, India

<sup>b</sup> Department of Chemical Engineering, Jaypee University of Engineering & Technology, Guna, A.B. Road, Raghogarh, Guna 473226, MP, India

## ARTICLE INFO

### Article history:

Received 6 March 2014

Received in revised form 19 August 2014

Accepted 22 September 2014

Available online 12 October 2014

### Keywords:

Multicomponent diffusion

Thin film

Free-volume theory

Skinning

## ABSTRACT

A simulation study on multicomponent polymeric solvent casting process was carried out using known different models and their relative performance of the model assessed in terms of residual parameters and solvent concentration profiles in the coating film. While all the models were found to predict nearly identical concentration profile for highly volatile solvents, significant variation in the profiles was observed in case of the less volatile solvents. Estimated values of the preexponential factors ( $D_{01}$  and  $D_{02}$ ) exhibited marginal differences implying perhaps a material balance deviation of the predictive models. The effect of air flow rate used for the drying process has been realized through its influence on the skinning behavior, low flow rate being the preferred while for maintaining the appropriate level of skinning.

© 2014 Elsevier B.V. All rights reserved.

## 1. Introduction

To produce the polymer coating, the casting of continuous layer of polymer solution is done on the substrate. These coatings are used in synthetic fiber, photographic films, magnetic media, etc. Photographic films, adhesives, image media, and magnetic media are different kinds of films which are made using thin film coating and drying technology. Drying is the last and quality controlling step in the polymeric coating. Drying conditions: air flow, oven temperature, and residence time, are responsible for final structure and properties of the coatings. Due to poor drying conditions, sometimes improper drying takes place, hence low quality, internal gradients, phase separations, colloidal transformations lead to wrong microstructure, inappropriate non-uniformities and stress related defects [1]. Simultaneous heat and mass transfer operations occur during the removal of volatile excess solvents from the coating [2]. The rate controlling step for drying shifts from external mass transfer to internal mass transfer within the coating, as the solvents evaporate. Diffusion and diffusion induced convection are responsible to move the solvents from the coating to the surface. Diffusion coefficient drops dramatically as the solvent concentration falls in case of polymeric coating [1]. The concentration of the solvent at the exposed surface drops during the course of drying. Hence, the drying rate falls steadily. This period is called falling rate

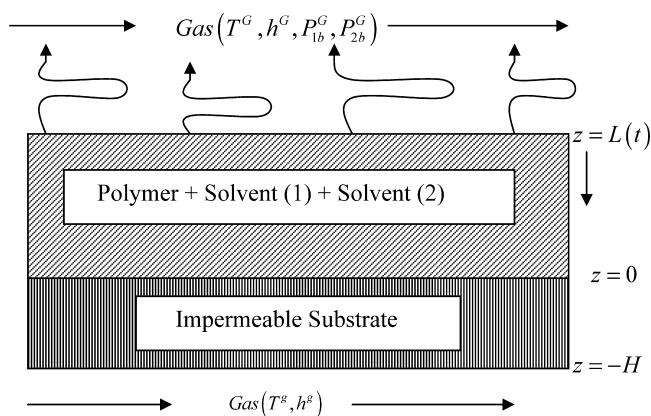
period. The diffusion coefficient of solvent in the polymeric coating is the strong function of the solvent concentration, temperature and molecular size.

In literature, several studies are reported for binary polymer–solvent coatings. The results of binary diffusion models compare well with experimental weight loss data [3–5]. Recently, the results of the binary model have been shown to compare well with depth profile measurements using confocal laser Raman spectroscopy [6]. All the multicomponent diffusion models [2,7–9] have been developed using Bearman's friction factor theory by making some assumptions. Therefore, a comparative study of these models is required to find the suitable model for the prediction of drying behavior in multicomponent coatings. Only few studies [2,10] have been reported in literature in this field. Schabel et al. [11] have modified the Flory–Huggins theory and found good agreement with experimental and model predicted diffusion data in case of poly (vinyl acetate)–methanol–toluene system. They have not shown the comparison among the different multicomponent diffusion models.

Recently, Arya and Vinjamur [12] have tested these diffusion models against the measured concentration profiles during drying. They have measured concentration profiles in ternary polymer–solvent–solvent systems using confocal Raman spectroscopy. They have compared measured profiles with model predicted values and found that none of multicomponent diffusion model is able to predict complete concentration profiles for the less volatile solvent. However, predictions of generalized model are much better than the Alsoy and Duda [2] and Zielinski and Hanley [8] models. Therefore, a comprehensive simulation study is needed

\* Corresponding author. Tel.: +91 175 2393444; fax: +91 175 2393005.

E-mail addresses: [rajaryache@gmail.com](mailto:rajaryache@gmail.com), [rajarya@thapar.edu](mailto:rajarya@thapar.edu) (R.K. Arya), [chitreshbhargava29@gmail.com](mailto:chitreshbhargava29@gmail.com) (C.K. Bhargava).



**Fig. 1.** Schematic of a drying coating.  $h^s$ : heat transfer coefficients at the base side,  $h^G$ : heat transfer coefficients at the surface of the coating,  $p_{1b}^G$ : partial pressure of solvent  $i$  in the bulk gas,  $L$ : thickness of coating, cm,  $t$ : time, s,  $z$ : thickness of the coatings at time  $t$ ,  $T^G$  and  $T^s$ : gas/air temperature at top and bottom sides respectively.

to study various multicomponent free volume diffusion models and their limitations. In this paper, a simulation study in ternary coating of one polymer and two solvents using all the available free volume theory models have been reported.

## 2. Model equations

**Fig. 1** shows the schematic of a drying coating, which has been cast on impermeable substrate. As soon as the solvent reaches the surface, it evaporates into the air on the top side of the coating. Then the mass of solvents decreases with time and coating–gas interface moves closer to the substrate opposite to diffusion. There is no mass transfer from the substrate side and hence the fluxes will be zero at the substrate.

### 2.1. Mass transport

Both the solvents are diffusing within the coating from substrate side to the coating side. At anytime total mass transfer of any diffusing species is the sum of the mass transfer due to its own concentration gradient and mass transfer due to concentration gradient of second solvent. The reference velocity is chosen to be volume average velocity because it is shown to be equal to zero if there is no change in volume on mixing [13].

Mass balance for solvent 1

$$\frac{\partial c_1}{\partial t} = \frac{\partial}{\partial z} \left( D_{11} \frac{\partial c_1}{\partial z} \right) + \frac{\partial}{\partial z} \left( D_{12} \frac{\partial c_2}{\partial z} \right) \quad (1)$$

Mass balance for solvent 2

$$\frac{\partial c_2}{\partial t} = \frac{\partial}{\partial z} \left( D_{21} \frac{\partial c_1}{\partial z} \right) + \frac{\partial}{\partial z} \left( D_{22} \frac{\partial c_2}{\partial z} \right) \quad (2)$$

$c_i$  is the concentration of solvent  $i$  ( $i=1,2$ ),  $t$  is the time,  $z$  is the thickness of the coatings at anytime,  $D_{11}$  and  $D_{22}$  are main diffusion coefficients that characterize transport due to solvents own concentration gradient,  $D_{12}$  and  $D_{21}$  are cross diffusion coefficients that characterize transport due to other solvents concentration gradient.

The concentration of polymer, balancing component, can be obtained by equating sum of mass fraction to one.

Mass fraction of solvent 1

$$\omega_1 = \frac{c_1}{c_1 + c_2 + (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer}},$$

$\omega_i$ : mass fraction of species  $i$ ,  $c_i$ : concentration of species  $i$ ,  $\hat{V}_i$ : specific volume of species  $i$ ,  $\rho_{polymer}$ : density of polymer.

Mass fraction of solvent 2

$$\omega_2 = \frac{c_2}{c_1 + c_2 + (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer}}$$

Mass fraction of polymer 3

$$\omega_3 = 1 - \omega_1 - \omega_2$$

But mass fraction of polymer can be calculated using,

$$\omega_3 = \frac{c_3}{c_1 + c_2 + (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer}}$$

Now equating mass fractions of polymer,

$$\begin{aligned} 1 - \frac{c_1}{c_1 + c_2 + (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer}} \\ - \frac{c_2}{c_1 + c_2 + (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer}} \\ = \frac{c_3}{c_1 + c_2 + (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer}} \\ \Rightarrow c_3 = (1 - c_1 \hat{V}_1 - c_2 \hat{V}_2) \rho_{polymer} \end{aligned} \quad (3)$$

Several theories for predicting main-term and cross-term diffusion coefficients have appeared in the literature. The theories begin with Bearman's statistical mechanical theory [14] that relates gradient of chemical potential of a species to frictional motion between the species and others of the system.

$$\frac{\partial \mu_i}{\partial z} = \sum_{j=1}^n c_j \xi_{ij} (v_i - v_j) \quad (4)$$

$(\partial \mu)/(\partial z)$  is chemical potential gradient;  $c_i$ , concentration of component  $i$ ;  $M_i$ , molecular weight of component  $i$ ;  $\xi_{ij}$  is friction coefficient between component  $i$  and  $j$ ;  $v_i$  and  $v_j$  are the mean velocities of component  $i$  and  $j$  respectively.

According to Bearman, self diffusion coefficients are also related to friction is given by

$$D_i = \frac{RT}{\sum_{j=1}^n (c_j/M_j) \xi_{ij}} \quad (5)$$

$D_i$  is self diffusion coefficient of species  $i$ ,  $R$  is universal gas constant and  $T$  is absolute temperature. Friction factors  $\xi_{ij}$  cannot be measured directly. Different assumptions on them led to different theories for diffusion in multicomponent mixtures.

Zielinski and Hanley [8] related chemical potential gradient to mass average velocity and frictional force experienced by the molecule. They related the mass flux with respect to volume average velocity to the mass flux with respect to the mass average velocity. Mass flux with respect to mass average velocity is related to frictional force experienced by a molecule. They assumed ratios of friction factors equal to the ratios of molecular weight. Mass average velocity is chosen as the reference velocity in their work. Model equations for their case are given in Table 1.

Dabral [9] modeled diffusive flux to the volume average velocity. He assumed friction between the solvents is equal ( $\xi_{12} = \xi_{21}$ ).

Download English Version:

<https://daneshyari.com/en/article/7107098>

Download Persian Version:

<https://daneshyari.com/article/7107098>

[Daneshyari.com](https://daneshyari.com)