



Mutual diffusion coefficients of *n*-butanol + *n*-heptane and *n*-pentanol + *n*-heptane from 288.15 K to 318.15 K



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ARTICLE INFO

Article history:

Received 16 November 2016

Received in revised form 9 May 2017

Accepted 23 May 2017

Available online 25 May 2017

Keywords:

Mutual diffusion coefficient

n-Butanol

n-Pentanol

n-Heptane

ABSTRACT

The mutual diffusion coefficients of *n*-butanol + *n*-heptane and *n*-pentanol + *n*-heptane were measured over the mass fraction of *n*-butanol or *n*-pentanol from 0.05 to 0.95 at intervals of 0.10 and the temperatures 288.15 K, 298.15 K, 308.15 K and 318.15 K at 0.101 MPa. The measurements were carried out using a digital holographic interferometry system. The expanded relative uncertainty of the mutual diffusion coefficients was estimated to be less than 2.4%. The influences of temperature and composition on the mutual diffusion coefficients were investigated. Moreover, equations for the mutual diffusion coefficients of the two binary mixtures were fitted to the data as functions of mass fraction and temperature. The correlations represent the data with the absolute average of relative deviations (AARDs) of 1.1% for *n*-butanol + *n*-heptane and 0.77% for *n*-pentanol + *n*-heptane, respectively.

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1. Introduction

Alcohols have been suggested as fuel additives, which can significantly enhance the octane rating, reduce the exhaust emissions of diesel engine and improve the combustion efficiency [1,2]. Compared with ethanol, *n*-butanol and *n*-pentanol have higher energy density, lower hygroscopicity, and lower volatility [3]. Recently, there has been increased interest in the performance and emission characteristics of diesel engines operating with *n*-butanol/diesel or *n*-pentanol/diesel fuel [1,4–6]. *n*-Butanol and *n*-pentanol are also used as cosolvents [7] and hydrophobic solvents [8].

As for the complex compositions of diesel oil, *n*-heptane, which has a cetane number and combustion characteristics similar to diesel oil, is usually considered as the standard substances substituted for diesel oil in experimental and theoretical combustion studies [9,10]. In recent years, many studies have focused on the thermodynamic properties and transport properties of *n*-butanol + *n*-heptane or *n*-pentanol + *n*-heptane mixtures, including vapor-liquid equilibria [11,12], excess molar volume [13,14], density [14,15], viscosity [15,16], speed of sound [17] and limiting activity coefficients [18].

Mutual diffusion is one of the most essential transport properties, critical for investigating the mass transfer mechanism for catalytic reactions and separation processes [19,20]. Moreover, accurate knowledge of the mutual diffusion coefficients of fuel or fuel additives are necessary to study and optimize spray, atomiza-

tion and combustion processes [21]. Nevertheless, there are no available reports on the mutual diffusion coefficients of *n*-butanol + *n*-heptane and *n*-pentanol + *n*-heptane up to now. Therefore, this work was undertaken to investigate the mutual diffusion coefficients of *n*-butanol + *n*-heptane and *n*-pentanol + *n*-heptane.

The diffusion behaviors of some alcohol + alkane binary mixtures have been studied, such as [22,23]. Previously, our group has investigated the mutual diffusion coefficients of isopropanol + *n*-heptane and isobutanol + *n*-heptane at temperatures from 288.15 K to 323.15 K by the digital holographic interferometry method [24]. In this work, the mutual diffusion coefficients of *n*-butanol + *n*-heptane and *n*-pentanol + *n*-heptane are measured at temperatures from 298.15 K to 318.15 K and pressure 0.101 MPa, mass fractions from 0.05 to 0.95 at intervals of 0.10. The effects of composition and temperature on the mutual diffusion coefficients are discussed.

2. Experimental section

2.1. Samples

All chemicals were supplied by Aladdin Reagent Inc. The chemicals were not further purified. The specified mass fractions for all chemicals are higher than 0.995 (GC) as stated by the supplier. Specifications of the samples are listed in Table 1. An electronic balance (ME204, Mettler Toledo, uncertainty is 0.2 mg) was used to prepare the binary mixed sample.

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Table 1

Selected physical and chemical properties of the samples used in this work.

Chemical	CAS number	Molecular weight/g.mol ⁻¹	Purification method ^a	Mass purity ^b	Supplier
<i>n</i> -Butanol	71-36-3	74.12	None	>0.995	Aladdin
<i>n</i> -Pentanol	71-41-0	88.15	None	>0.995	Aladdin
<i>n</i> -Heptane	142-82-5	100.20	None	>0.995	Aladdin
Potassium Chloride	7447-40-7	74.45	None	>0.995	Aladdin
Water	7732-18-5	18.02	None	>0.999	Aladdin

^a No further purification.^b As stated by the supplier.

2.2. Measurement theory and apparatus

There are many different techniques for measuring mutual diffusion coefficients. The most accurate measurement methods are Gouy interferometry [25,26] and Rayleigh interferometry [27,28]. Holographic interferometry is also widely used to measure mutual diffusion coefficients [29–32].

In this work, the digital holographic interferometry method was used to measure the mutual diffusion coefficients. A complete and more detailed description of the measurement principle and our apparatus can be found in our previous papers [33–35] and various fundamental studies [29–32]. Here only brief description is presented.

The fundamental theory of digital holographic interferometry is based on Fick's second law for one-dimensional diffusion, which can be written as

$$\left(\frac{\partial c}{\partial t}\right) = D_{12} \left(\frac{\partial^2 c}{\partial z^2}\right) \quad (1)$$

where D_{12} is the mutual diffusion coefficient, t is the diffusion time, c is the sample concentration and z is the diffusion direction. From an analysis of the linear relationship between the variations of the object beam phase with the concentration, D_{12} can be deduced as

$$D_{12} = \frac{\Delta z_m^2 [(1/t_1) - (1/t_2)]}{8 \ln(t_2/t_1)} \quad (2)$$

where t_1 and t_2 are two different diffusion times in the diffusion process, Δz_m is the distance between the two extreme points of the solution's concentration differences. As it is difficult to confirm the initial time of the diffusion process, the parameter t_0 named as zero time was introduced to correct t_1 and t_2 , as described in Ref. [36]. Eq. (2) can be expressed as

$$D_{12} = \frac{\Delta z_m^2 [1/(t_1 + t_0) - 1/(t_2 + t_0)]}{8 \ln[(t_2 + t_0)/(t_1 + t_0)]} \quad (3)$$

Eq. (3) is the final equation for measuring the mutual diffusion coefficient. The diffusion time t_1 and t_2 can be obtained from the computer hardware clock. The distance between the maximum and minimum of the concentration difference (two peaks in the concentration difference profiles, Δz_m) can be obtained from the holographic interferograms at t_1 and t_2 . For the known t_1 and t_2 , the value of Δz_m is constant. The nonlinear transcendental equations can be established in terms of t_1 , t_2 and Δz_m . Then the mutual diffusion coefficient D_{12} can be calculated. Fig. 1 shows a typical digital image processing which was used to obtain Δz_m .

Fig. 2 shows the optical system of digital holographic interferometer employed for the mutual diffusion coefficient measurements. A He–Ne laser (15 mW, 632.8 nm) was used as the light source. The rectangular diffusion cell measures 1.2 cm × 1.2 cm × 6 cm. A CCD camera (1024 × 1024 pixels, 7.4 × 7.4 μm pixel size) was used to acquire the holographic image. The diffusion cell was immersed in a water bath (JULABO F33-ME) to maintain the constant temperature of sample. Temperature fluctuations in the

water bath were within ±0.02 K. A platinum resistance thermometer (PRT, Fluke 5608-12) was used to measure the temperature with an uncertainty of ±0.01 K. The pressure was measured by a pressure transmitter (Rosemount 3051 s) with an uncertainty of ±5 kPa.

3. Uncertainty evaluation

The uncertainty evaluation is listed in Table 2. The uncertainty of the temperature results from the uncertainties of the platinum resistance thermometer readings, the temperature stability of the system and the platinum resistance thermometer measurement circuit. The standard uncertainty in temperature is $u(T) = 0.021$ K. The uncertainty of pressure is composed of the uncertainties in pressure transmitter and pressure measurement circuits, the standard uncertainty in pressure is $u(p) = 0.005$ MPa.

The mass fraction w_i is calculated by

$$w_i = \frac{m_i}{m_1 + m_2} \quad (4)$$

where w_i , m_i are the mass fraction and mass of component i , respectively. The combined relative standard uncertainty of mass fraction is given by

$$u_r(w) = \sqrt{\left(\frac{\partial w_1}{\partial m_1}\right)^2 u_1^2 + \left(\frac{\partial w_2}{\partial m_2}\right)^2 u_2^2 + u_r^2(i_1) + u_r^2(i_2)} \quad (5)$$

where u_1 and u_2 are the uncertainties of m_1 and m_2 , $u_r(i_1)$ and $u_r(i_2)$ are the uncertainties caused by purity of chemicals. The uncertainty caused by impurity was considered according to GUM 1995 [36]. With a purity of 0.995, the relative standard uncertainties caused by purity

$$u_r(i) = 0.005/\sqrt{3} \approx 0.003 \quad (6)$$

The relative expanded uncertainty in mass fraction can be calculated from $U_r(w) = k \cdot u_r(w)$, which was 0.008 with the coverage factor $k = 2$ (0.95 level of confidence).

The uncertainty in the mutual diffusion coefficient is composed of the uncertainties in diffusion time t (t_1 and t_2) and the distance between the maximum and minimum of the concentration difference Δz_m . The combined relative standard uncertainty in the mutual diffusion coefficient is estimated by

$$u_r(D_{12}) = \sqrt{\sum_{i=1}^2 \left(\frac{\partial D_{12}}{\partial t_i}\right)^2 u^2(t_i) + \left(\frac{\partial D_{12}}{\partial (\Delta z_m)}\right)^2 u^2(\Delta z_m)} \quad (7)$$

The relative expanded combined uncertainty of mutual diffusion coefficient is 2.4% with the coverage factor $k = 2$ (0.95 level of confidence).

4. Results and discussion

The accuracy and reliability of our experimental system was verified by measuring the mutual diffusion coefficient of

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