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Mutual diffusion behavior of short chain alcohols + *n*-octane mixtures

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ABSTRACT

Mutual diffusion coefficients of several short chain alcohols (ethanol, *n*-propanol and *n*-butanol) + *n*-octane mixtures in the temperature range from 283.2 K to 313.2 K at different concentrations were measured using holographic interferometry. The relation between the mutual diffusion coefficient with temperature, viscosity, concentration and molecular weight is investigated, respectively. The Onsager–Fuoss model is applied to analyse the various influence factors. A new correlation taking into account the effect of the temperature and concentration on the mutual diffusion coefficient is proposed to fit well the experimental data.

1. Introduction

Biodiesel mainly refers to the fatty acid monoalkyl ester produced by the transesterification of the grease, vegetable oils or animal fats with short chain alcohols. It has been proven to be a promising alternative fuel for diesel engine. Compared with traditional fuels, it has lots of advantages: excellent environmental performance, low-temperature startup, stability, renewability and so on [1,2]. But in the production of biodiesel the grease and alcohols are not miscible with each other, and the mass transfer is limited. The immiscibility will leads to the formation of two phases and so the reaction only takes place in the interphase boundary, which will result in a obvious drop in the reaction conversion and reaction rate [3]. This problem can be overcome by the addition of the cosolvent in reaction system. The cosolvent helps to create a single homogeneous phase of the grease and alcohols, and greatly accelerates the reaction conversion and reaction rate [4,5]. The cosolvent used in the production of biodiesel mainly includes the following categories: (i) alkanes and cycloalkanes; (ii) ketone; (iii) ether; (iv) alcohols; (v) other common solvents [6].

The mutual diffusion coefficients of short chain alcohols + cosolvent mixtures strongly affect the catalytic reaction and separation processe in the production of biodiesel [7,8]. The accurate data is used for predicting the rate-limiting factors in chemical reaction and further optimizing the design of processing equipment. Bosse et al. [9] measured the mutual diffusion coefficients of alcohols + *n*-hexane and alcohols + cyclohexane at 298.15 K over the whole concentration range; Ramakanth et al. [10] measured the mutual diffusion coefficients of alcohols + cyclohexane at 298.15 K and different concentrations. *n*-Octane, one kind of alkanes, has attracted the increasing interest as an excellent cosolvent in the production of biodiesel [8]. But there are no the mutual diffusion coefficient data of short chain alcohols + *n*-octane.

Therefore, in this work, the mutual diffusion coefficients of different short chain alcohols (ethanol, *n*-propanol and *n*-butanol) + *n*-octane mixtures were measured by holographic interferometry. The mass fraction and temperature range are from 0.1 to 0.9 and from 283.2 K to 313.2 K, respectively. The relation between the mutual diffusion coefficient with temperature, viscosity, concentration and molecular weight is investigated, respectively. A new correlation was presented for the experimental data.

2. Experimental

2.1. Materials

All chemicals in this work were supplied by Aladdin Industrial Corporation and used without any further purification. Table 1 presented molecular formula, molecular weight and purities of the chemicals. For the sample preparation, the chemicals were

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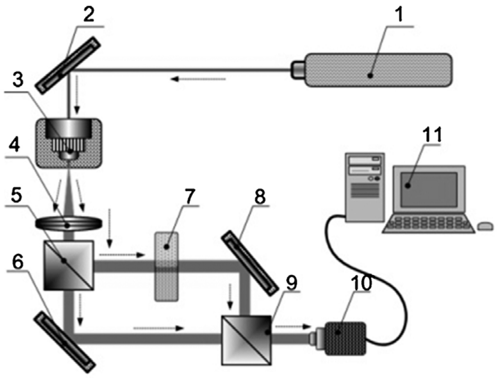


(1) He–Ne laser, (2) mirror, (3) spatial filter, (4) collimating lens, (5) beam splitter, (6) mirror, (7) diffusion cell,
(8) mirror, (9) beam splitter, (10) CCD camera, (11) computer

Fig. 1. Optical system of holographic interferometry.

Table 1
Description of the chemical samples.

Chemical	CAS no.	Molecular weight (g mol^{-1})	Purification method[a]	Mass fraction purity[b]	Supplier
n-Octane	111-65-9	114.22	None	>0.995	Aladdin
Ethanol	64-17-5	46.07	None	>0.997	Aladdin
n-Propanol	71-23-8	60.07	None	>0.997	Aladdin
n-Butanol	71-36-3	74.12	None	>0.997	Aladdin
Potassium chloride	7447-40-7	74.45	None	>0.995	Aladdin
Water	7732-18-5	18.02	None	Deionised ultra-pure water	Our laboratory

[a] No further purification.
[b] As stated by the supplier.

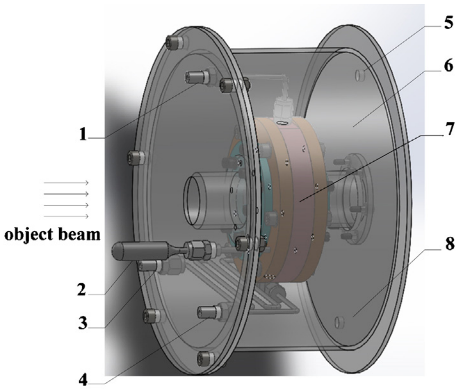
weighted by an electronic balance (Shanghai Shunyu FA2004, uncertainty: 0.1 mg). Two chemicals are thoroughly stirred in a 100 mL reagent bottle, and then let them stand for about 24 h before using them.

2.2. Experimental system

Fig. 1 shows the schematic of the holographic interferometry experimental system which has been reported in previous work [11,12]. The experimental system mainly consisted of optic interference system, diffusion cell system and image acquisition and processing system. The optical components and diffusion cell are placed on the vibration isolator table to reduce the environmental vibration.

In this work, a Mach–Zehnder interferometer is employed as shown in Fig. 1. The light from a He–Ne laser (15 mW, 632.8 nm) is expanded by a spatial filter, and collimated by a collimating lens to get a wider field of view. With a beam splitter the beam is split into the object beam passing through the diffusion cell and the reference beam. The object beam and the reference beam are joined by a second beam splitter and interfere in the front of the CCD camera.

The diffusion cell system is shown as Fig. 2. A diffusion cell measured 1.2 cm × 1.2 cm × 6 cm is constructed so that the diffusion can be regarded as the one-dimension process. The cell is sandwiched between two pieces of quartz glass windows to allow the beam to pass through. To create good boundary conditions, some capillary tubes are equipped in the diffusion cell. The whole cell is first filled with the lighter solution (lower density), and then the heavier solution (higher density) is slightly injected until the diffusion interface reaches the middle of the cell. The flow rate of the solution is suitable to avoid the turbulence of the solution. The temperature of the diffusion cell is controlled by a constant temperature water bath (JULABO F33-ME, uncertainty: ±0.1 K) and recorded by a Keithley 2700 digital multimeter with a temperature transducer Pt100 (Fluke 5608–12 PRT, uncertainty: ±0.02 K).



(1) liquid outlet, (2) Pt 100, (3) liquid inlet, (4) liquid outlet, (5) outlet for water bath,
(6) water bath, (7) diffusion cell, (8) inlet for water bath

Fig. 2. Diffusion cell system.

The software was developed by MATLB for the image acquisition and processing [11]. The holographic interferograms were recorded every 5 min as shown in Fig. 3(a). With Fourier transform, the spectrogram included the phase and amplitude in frequency domain was picked up and is described by the bright part of Fig. 3(b). Then the inverse Fourier transform is used to obtain the phase information of the object beam as shown in Fig. 3(c). We can get the wrapped phase difference by analysing the phase information at different time t_1 and t_2, which is shown in Fig. 4(a). The continuous phase difference was got by unwrapping the wrapped phase difference as shown in Fig. 4(b). A polynomial is used to fit the continuous phase difference in the y-directions. The dependency of the