International Communications in Heat and Mass Transfer 76 (2016) 225–236

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

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

Accurate measurement of temperature and concentration distribution of a mixture in a rectangular parallelepiped enclosure☆

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ARTICLE INFO

Available online 26 May 2016

Keywords:
Mach–Zehnder interferometer
Diffusion
Soret effect

ABSTRACT

Thermal diffusion in the 50/50 wt.% binary hydrocarbon mixture of 1,2,3,4-tetrahydronaphthalene (THN)/dodecane (C_{12}) at a mean temperature of 298 K was studied experimentally in two cells with different geometries. The thermal design of the geometries was investigated numerically, and the effect of the location of the filling channel was studied. The newer design showed a more linear temperature profile with smaller values of velocity than the earlier design. The thermal experimental results were in agreement with the numerical calculations. Unlike the previous design, the segregation of the components in the new design was not affected by convective motions, and the calculated Soret coefficient agreed with the benchmark values.

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1. Introduction

Fickian diffusion occurs in any multicomponent liquid mixture that has a concentration gradient. However, diffusion can also happen in a mixture without a concentration gradient if there is a thermal gradient present. This sort of diffusion where separation of the components is induced by the thermal gradient is named thermal diffusion, thermodiffusion, or the Soret effect. This effect has been used in various fields of study. For instance, it has been utilized to separate biological particles such as bacteria [1] and colloidal particles [2]. It has been also used for trapping DNA [3], and it is very important in the oil industry since distributions of the components in the hydrocarbon mixtures in oil reservoirs are affected by thermal diffusion [4–6].

There are several experimental techniques that can be implemented to study the Soret effect in liquid mixtures. Rahman and Saghir [7] presented a historical review of experimental and theoretical approaches to investigate the Soret effect. Platten [8] suggested two general categories of these techniques: (1) convective coupling systems and (2) convectionless systems.

In the convective coupling techniques, the changes in the velocity field due to thermal diffusion are measured. The Rayleigh–Bénard configuration [9] and the thermogravitational column (TGC) [10–17] are examples of convective coupling techniques.

In convectionless systems, convective motions must be avoided. In a classic Soret cell, the mixture is contained in a cubic cavity. The side walls are made of materials with low heat conductivity to avoid lateral heat transfer. The upper and lower walls of the cavity are bounded by copper plates with constant temperatures. The system remains hydrodynamically stable if it is heated from above. By applying a temperature gradient, the components segregate due to the Soret effect.

The mass flux in a binary mixture is described by:

$$J = -\rho D_M \nabla C - \rho D_T C_0 (1 - C_0) \nabla T \tag{1}$$

where ρ stands for the density, C is the concentration, D_M is the molecular diffusion coefficient, C_0 is the initial concentration, and D_T stands for the thermal diffusion coefficient. In Eq. (1) on the right hand side, the first term represents the Fickian diffusion and the second term represents the diffusion due to the Soret effect. When the system reaches steady state, samples are taken from points near the hot and cold sides of the cell to measure the concentration values and find the concentration gradient between the hot and cold sides. In the steady state, where the mass flux is zero, Eq. (1) becomes

$$\nabla C = -\frac{D_T}{D_M} C_0 (1 - C_0) \nabla T \tag{2}$$

where ∇C represents the concentration gradient between the two measured points, ∇T is the temperature difference between those points, and $\frac{D_T}{D_M}$ is the Soret coefficient, S_T, which can be alternatively obtained from

$$S_T = -\frac{1}{C_0(1 - C_0)} \frac{\nabla C}{\nabla T} \tag{3}$$

Optical measurement techniques are widely used to conduct thermodiffusion experiments using a modified classic Soret cell. The

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☆ Communicated by W.J. Minkowycz.

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http://dx.doi.org/10.1016/j.icheatmasstransfer.2016.05.020
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Nomenclature

C_i	Mass fraction of mixture component *i*
C_0	Initial mass fraction
C_P	Specific heat capacity (J g^{-1} k^{-1})
D_M	Isothermal molecular diffusivity (cm^2 s^{-1})
D_T	Thermodiffusion coefficient (cm^2 s^{-1} k^{-1})
g	Gravitational acceleration (cm s^{-2})
h	Height of the cell (mm)
J_i	Molar flux of mixture component *i* (J cm^2 cm^{-1})
K	Thermal conductivity (J s^{-1} cm^{-1} k^{-1})
n	Index of refraction (−)
P	Pressure (Pa)
P_{atm}	Atmosphere pressure (Pa)
S_T	Soret coefficient (K^{-1})
T	Temperature (K)
T_{amb}	Ambient temperature (K)
u	Velocity component in *x* direction (cm s^{-1})
v	Velocity component in *y* direction (cm s^{-1})
Greek symbols	
μ	Dynamic viscosity (Pa s)
ρ	Density (g cm^{-3})
τ_{th}	Thermal characteristic time (s)
τ_D	Diffusion characteristic time (s)
θ	Inclination angle (°)

beam deflection technique (BDT) is an example [18,19]. In this method, a laser beam passes through the transparent liquid mixture and is deflected due to the distribution of the temperature and concentration fields. The deflected laser beam is imaged and recorded by a CCD camera. Thereafter, differences in temperature and concentration are extracted by processing the captured images. The lateral walls of the modified classic Soret cell used in this technique are made of quartz glass in order to be transparent to the laser beams.

Another optical technique with high reliability is optical digital interferometry (ODI). The non-intrusive nature of this method is amenable to convectionless systems. One of the distinctive features of this technique is its ability to measure the transient temperature and concentration fields during the experiment. Rahman and Saghir [20] have used this method to measure the Soret coefficients of binary hydrocarbon mixtures in a cubic cavity.

Although convectionless techniques have been popular for thermodiffusion experiments, most of the research has suffered from the presence of deleterious convections. Some studies were done to overcome the problem [21,22].

To the best of our knowledge, so far no study has been done on the effect of the location of the filling channel (injection hole) on the convections in the mixture. In the present study, thermal diffusion in a binary mixture was studied in two Soret cells with different geometries. The first geometry was that of a classic Soret cell. The effect of the location filling channel was studied numerically in this cell, which then led us to design a new cell to minimize unwanted convections. The numerical results showed a significant decrease of the convections in the newly designed cell. Then, the new cell was prepared for experimental measurements using the ODI technique. The fluid used in the experiments was the benchmark mixture of THN–C_{12} at 50 wt.% of concentration and a mean temperature of 298 K. The fast Fourier transform (FFT) method was used for image processing of the fringes obtained from the interferometry technique. The new cell was proved to be well-optimized with less convection, and it will be prepared for testing with a ternary mixture in the future.

2. Experimental setup and procedure

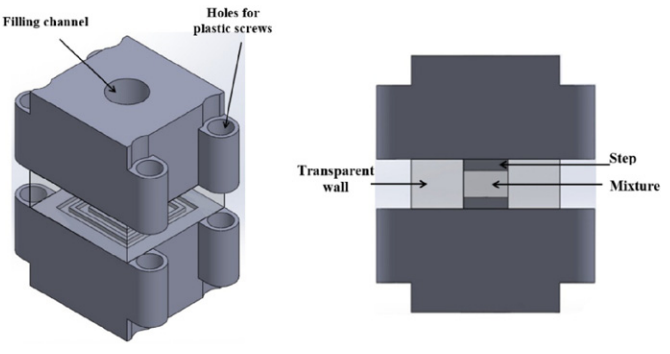
Two Soret cells with different dimensions and geometries were used in the present study. Both geometries are explained here in detail.

2.1. Description of the first design

The schematic of the first cell (the classic design) is shown in Fig. 1. It consisted of two nickel-plated copper blocks with dimensions of $30 \times 30 \times 20\,\text{mm}^3$ where the height was 20 mm. A cubic cavity with quartz walls was enclosed between the two blocks. The mixture was placed in this cavity. The width and length of the glass frame were equal to those of the copper block, and the height was 10 mm. The dimensions of the cavity were $10 \times 10 \times 10\,\text{mm}^3$. On one side of each copper block a step with height of 2.5 mm was provided which enters the glass frame. Thus, the total height of the mixture enclosed in the cavity was 5 mm. The aspect ratio (length/height) was two. Two concentric N-Buna O-rings with different diameters were used on each side of the frame in contact with the blocks to seal the cell. A filling channel with diameter of 1 mm was provided in the centre of the blocks. After filling the cell with the mixture, the blocks were sealed with screw plugs. There was a hole on the side of the blocks where a thermistor was inserted to measure the temperature near the plate in contact with the mixture. To clamp the frame between the blocks and assemble the cell, four plastic screws were used. There was no heat insulation material used for this cell.

2.2. Description of the second design

In the second design (the new design), the steps on the plates were removed and the glass frame was clamped between the flat plates. The dimensions of the copper blocks were the same as those in the previous design. The size of the cavity was $15 \times 15 \times 2.5\,\text{mm}^3$where the height is 2.5 mm, making the aspect ratio six. The filling channels were relocated to the corners of the block in order to reduce the convection effects in the centre of the mixture. This is discussed in more detail in Section 4.1. Instead of using plastic screws, polytetrafluoroethylene (PTFE) walls were used to assemble the cell. The dent on top of the each block allowed the PTFE walls to secure the blocks and glass frame in place. Moreover, these walls insulated the cell and prevented the heat transfer between the cell and the environment. In order to allow the laser beams to pass into the cell, windows were provided on the front and back walls. The holes for mounting thermistors could be placed closer to the mixture than in the classic cell, since the protrusions on the blocks were removed. Therefore, the temperature read by the sensors was more accurate in the new design. The cross-sectional view of the cell illustrated in Fig. 2 shows all of the relevant details of the new design.



(a) isometric view (b) side view

Fig. 1. Side view of the classic cell.

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