Thermochimica Acta 560 (2013) 63–70

Contents lists available at SciVerse ScienceDirect

Thermochimica Acta

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

Heat capacity, thermal conductivity and thermal diffusivity of aqueous sulfolane solutions

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ARTICLE INFO

Article history:
Received 17 January 2013
Received in revised form 2 March 2013
Accepted 12 March 2013
Available online 21 March 2013

Keywords:
Heat capacity
Thermal conductivity
Thermal diffusivity
Sulfolane
Physical solvent

ABSTRACT

In this work, the thermal properties including molar heat capacity, thermal conductivity, and thermal diffusivity of aqueous sulfolane solutions were measured at temperatures ranging from (303.15 to 353.15) K and atmospheric pressure. The measurements were carried out for the entire range of mole fractions of sulfolane in water. Molar excess heat capacities as well as excess thermal conductivities and excess thermal diffusivities were calculated from the experimental values and correlated as a function of mole fraction and temperature using the Redlich–Kister equation. Employing the heat capacity, thermal conductivity and thermal diffusivity of pure water as the solvent, the corresponding experimental values obtained for the investigated solutions were also correlated with temperature and concentration by a modified Setchenow equation. Results show comparable accuracy of both models in correlating all three experimental thermal properties.

1. Introduction

Physical solvents such as sulfolane (SFL), 1-methyl-2-pyrolidinone (NMP) and *N*,*N*-dimethylformamid (DMF) are non-reactive, organic polar compounds, which physically dissolve acid gases. Because of their capability of removing acid gases such as CO_2 and H_2S from high-pressure gas streams, they are of industrial importance and have been the subject of extensive studies during the last 25 years [1,2]. Solvent regeneration is carried out in desorption stage of the process by reducing the pressure and requires less energy consumption than chemical solvents. Physical solvents are less corrosive than chemical solvents because no chemical reaction takes place with the acid gases.

Thermo-physical properties such as density, viscosity, surface tension, heat capacity, thermal conductivity and thermal diffusivity of pure physical solvents and their aqueous solutions, are necessary for the design of acid gas treatment equipment, especially those in which heat and mass transfer is important, as well as for measuring and interpreting other physicochemical properties.

Sacco et al. [3] reported the experimental densities and viscosities of water + sulfolane mixtures over the whole mole fraction range at temperatures 303.15 K, 313.15 K, and 323.15 K. Yu et al. [4] reported the densities of water + sulfolane as well as water + tetraethylene glycol and benzene + tetraethylene glycol mixtures over the entire concentration range at 298.15 K and atmospheric pressure by using an oscillating tube densimeter. Saleh et al. [5] reported the atmospheric pressure densities and viscosities of water + sulfolane mixtures in the entire composition range at temperatures ranging from (303.15 to 323.15) K. Steele et al. [6] reported heat capacity, vapor pressure, and density along the saturation line, measurements for cyclohexane-1-one, 1,2-dichloro-propane, 1,4-di-tert-butylbenzene, (±)-2-ethylhexanoic, 2-(methylamino)ethanol, perfluoro-n-heptane, and sulfolane. Castagnolo et al. [7] measured heat capacities of binary liquid mixtures of water–sulfolane and water–hexamethylphosphotriamide. Ho [8] reported heat capacity of aqueous solution for sulfolane and 2-amino-2-methyl-1-propanol (AMP) by differential scanning calorimeter and Mundhwa et al. [9] measured the heat capacity of water–SFL system at temperatures from (303.15 to 353.15) K. To the best of our knowledge, there is no information available in open literature concerning thermal conductivity and thermal diffusivity of aqueous SFL solutions.

In this work, the results of the measurement of thermal properties, i.e. molar heat capacity, thermal conductivity and thermal diffusivity of aqueous solutions of sulfolane by an absolute transient hot wire method at temperatures from (303.15 to 353.15) K and atmospheric pressure are reported. The obtained experimental data are correlated by a modified Setchenow equation as well as Redlich–Kister equation, and the results are also interpreted from molecular point of view.

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http://dx.doi.org/10.1016/j.tca.2013.03.017

2. Experimental

2.1. Materials

SFL (CAS Registry No. 126-33-0) was obtained from Aldrich Chemical Co. with a nominal mass purity > 99% and used without further purification. Water used as solvent was distilled deionized, which was degassed in an ultrasonic bath (FUNGILAB, model UA10MFD) at a temperature and wave frequency of 343 K and 50 kHz, respectively, for about 1 h prior to use. All solutions were prepared by measurement of mass of the solutes and solvent on a calibrated balance (Mettler model AE 200) with an uncertainty ±0.0001 g and measuring the volume of the solution by a standard volumetric flask up to 100 mL.

2.2. Apparatus and procedure

The measurements of heat capacity, thermal conductivity and thermal diffusivity were carried out using a PSL Systemtechnik instrument equipped with a Lambda measuring and evaluation system. The operation of the instrument is based on the in-stationary hot-wire resistance technique [10,11]. The hot-wire is made up of a thin platinum wire, which is soldered to the Lambda's sensor head. The sensor head contains a temperature sensor and they are altogether inserted into the liquid sample in the measurement cell. All wetted compartments of the apparatus (except hot wire) are constructed from 316L stainless steel. The hot-wire produces a constant heat stream to the surrounding liquid and at the same time it serves as the measuring sensor. To exclude convection influences, the temperature of the liquid sample was regulated to a very homogenous allocation by means of a precision thermostat unit (LabTemp model 300) and the measurements were carried out at minimum time intervals. The temperature stability of the precision thermostat was better than ±0.05 K. To obtain precise measurements of the thermal properties of samples, the temperature scale of the PSL Systemtechnik instrument was first calibrated for the temperature range (298.15–353.15) K. The heat capacity of the samples in the PSL Systemtechnik is measured on the basis of the operation of conventional calorimeters, which take advantage of the measurement of the voltage of an heating element of know or measureable resistance that a constant DC current passes through it followed by measurement of the increase in temperature of the sample, ΔT. After calibration and evaluation of the heat capacity of the calorimeter, the heat capacity of the samples can be measured.

It must be emphasized that the volume of the measurement cell was filled completely with the liquid sample and capped tightly with the sensor head. Therefore there was no vapor-phase space for the liquid phase to vaporize. This resulted in constant composition of the solutions during the course of the measurements. Also, it must be mentioned that the PSL Systemtechnik instrument is not able to directly measure the thermal diffusivity, but calculates this property from simultaneous measurement of heat capacity, thermal conductivity and the density of liquid samples using the well-known relation, $\lambda = \alpha\ \rho\ C_P$, where λ, α, ρ, and C_P stand for thermal conductivity, thermal diffusivity, density and heat capacity, respectively. In general, each reported data was an

Table 1
Review of the literature data for the molar heat capacity, thermal conductivity, and thermal diffusivity of pure water, toluene and sulfolane.

T/(K)	C_P/(J mol^{-1} K^{-1})		$10^3\ \lambda$/(W m^{-1} K^{-1})		$10^8\ \alpha$/(m^2 s^{-1})	
	This work	Lit (Ref.)	This work	Lit (Ref.)	This work	Lit (Ref.)
Water [12]						
303.15	75.30	75.301	613.7	615.50	14.75	14.790
313.15	75.26	75.294	630.7	630.62	15.22	15.207
323.15	75.30	75.328	643.7	643.59	15.59	15.578
333.15	75.39	75.393	654.8	654.38	15.91	15.904
343.15	75.48	75.485	663.2	663.12	16.20	16.186
353.15	75.60	75.605	670.0	670.01	16.43	16.428
ARD %	0.017		0.067		0.095	
MRD %	0.045		0.29		0.27	
Toluene						
303.15	159.8	158.21	129.4	129.54 [14]	8.598	8.592 [15]
308.15	160.9	159.72	127.5	128.03 [14]	8.466	8.453 [15]
313.15	162.8	161.24	125.7	126.52 [14]	8.349	8.317 [15]
318.15	164.0	162.79	124.2	125.03 [14]	8.230	8.183 [15]
323.15	165.7	164.35	123.3	123.54 [14]	8.066	8.051 [15]
328.15	167.1	165.93	122.3	122.06 [14]	7.993	7.922 [15]
333.15	168.8	167.53	121.1	120.59 [14]	7.905	7.796 [15]
338.15	170.2	169.15	118.6	119.14 [14]	7.786	7.672 [15]
343.15	171.5	170.78	117.0	117.71 [14]	7.669	7.551 [15]
348.15	173.1	172.43	115.9	116.30 [14]	7.570	7.432 [15]
353.15	174.9	174.09	113.5	114.90 [14]	7.382	7.316 [15]
ARD %	0.69		0.48		0.86	
MRD %	1.0		1.2		1.8	
Sulfolane						
303.15	181.5	182 [9]				
308.15	183.0	184 [9]				
313.15	185.1	185 [9]				
318.15	186.5	186 [9]				
323.15	188.7	188 [9]				
328.15	189.6	189 [9]				
333.15	192.3	191 [9]				
338.15	192.6	193 [9]				
343.15	194.3	194 [9]				
348.15	195.6	197 [9]				
353.15	197.8	199 [9]				
ARD %	0.38					
MRD %	0.72					