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Extended Abstract

Fluid properties simulation challenge Recommendations for problem III: viscosity of 2-propanol, *n*-nonane, and their mixtures☆

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Pure compounds		
Problem conditions	(a) 0.1 MPa, 300 K *n*-Nonane	(b) 0.1 MPa, 300 K 2-Propanol
Recommended values	0.650 ± 0.007 mPa s	1.986 ± 0.021 mPa s
Mixtures		
Problem conditions	(c) 0.1 MPa, 300 K $x = 0.5$, 2-propanol	(d) 0.1 MPa, 300 K $x = 0.75$, 2-propanol
Recommended values	0.756 ± 0.008 mPa s	1.040 ± 0.011 mPa s

Primary source of recommendation

All four values were obtained through from measurements performed for the Simulation Challenge at The Dow Chemical Company, Research and Development Department, Thermal Group. Experimental details are given below.

Justification for recommendation

Kinematic viscosity was determined from direct laboratory measurement by Ubbelohde capillary viscometer. Kinematic viscosity was converted to viscosity by multiplying by density which was measured by vibrating-tube densimeter.

Experimental details

Materials

The *n*-nonane (Aldrich 29,682-1; >99 mass %) and the 2-propanol (Aldrich 29,328-8; >99.5 mass %) were used as received. Karl–Fischer analysis gave 170 ppm-mass (0.017 %) water in the 2-propanol. Two mixtures were prepared gravimetrically: 50.01 mol.%, 2-propanol and 74.97 mol.% 2-propanol, compositions are reported here as mole fractions.

Apparatus[1]

Kinematic viscosities were measured with an Ubbelohde viscometer (Cannon Instruments Co.; Model 0C) [1] in a Cannon Model CT-1000 thermostat. The viscometers were

☆ This paper presents details of the determination of the recommended values used in the judging of problem III from the first Industrial Fluids Simulation Challenge.

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[1] In order to describe materials and experimental procedures adequately, it is occasionally necessary to identify commercial products by manufacturers' names or labels. In no instance does such identification imply endorsement by the National Institute of Standards and Technology, nor does it imply that the particular product or equipment is necessarily the best available for the purpose.

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Table 1
Experimentally determined density data for the subject fluids of Problem III

System[a]	Density ($kg\,m^{-3}$)
n-Nonane	712.33
2-Propanol	779.42
x =0.5, 2-propanol	728.73
x = 0.75, 2-propanol	746.31

[a] Temperature = 300 K; Pressure = 0.1 MPa.

calibrated by the manufacturer in 1998. Densities were measured in a Model DMA 58 Anton-Paar vibrating-tube densimeter [2] which had been calibrated with air and degassed HPLC water according to the manufacturer's procedure.

Temperatures in the thermostat were controlled to ±0.01 K. Temperatures were measured with a Model 1506 Hart Scientific 25 Ω platinum resistance thermometer calibrated by the manufacturer.

Procedure—viscosity

The laboratory procedure is described in ASTM method D 445, Standard Test Method for Kinematic Viscosity of Transparent and Opaque Liquids [3]. The kinematic viscosities were measured in quadruplicate.

Procedure—density

The laboratory procedure is described in ASTM method D 4052, Density and Relative Density of Liquids by Digital Density Meter [4]. The densities of the four fluids were measured in duplicate and are given in Table 1.

Estimation of uncertainty

Measurement uncertainties were appraised by adhering as closely as possible to NIST Technical Note 1297 [5]. However, as described in detail by Mandel [6], the evaluation of experimental measurements values is a difficult and ill-defined process in the absence of exactly-known reference values. In the rarely achieved absence of systematic errors, the uncertainty of experimental measurements should be of the same order as the precision (rms error) of replicate experiments. The rms errors among the four viscosity replicates at are ±0.002 mPa s (0.29%), ±0.011 mPa s (0.55%), ±0.005 mPa s (0.62%) and ±0.003 mPa s (0.31%) for parts (a), (b), (c), and (d) of the problem, respectively. The rms error between the two density replicates is 0.02 $kg\,m^{-3}$.

The typical uncertainty of kinematic viscosity measurements, given by the Precision and Bias statement of ASTM D 445 is ≈0.70%. This margin is based on periodical Interlaboratory comparisons (Round Robin). Also, in the absence of a verification of the manufacturer's calibration, ASTM D 445 indicates that an additional uncertainty allowance of 0.35% should be included.

The magnitude of the uncertainty of the viscosity data can be estimated from comparisons of the *n*-nonane and 2-propanol viscosity data available in the literature. A previously reported viscosity value for *n*-nonane [7] at 300 K, (0.652 mPa s), agrees with the contest measured value to within 0.40%. Fig. 1 shows an Arrhenius fit to the contest data and three sets of recently-reported data on 2-propanol

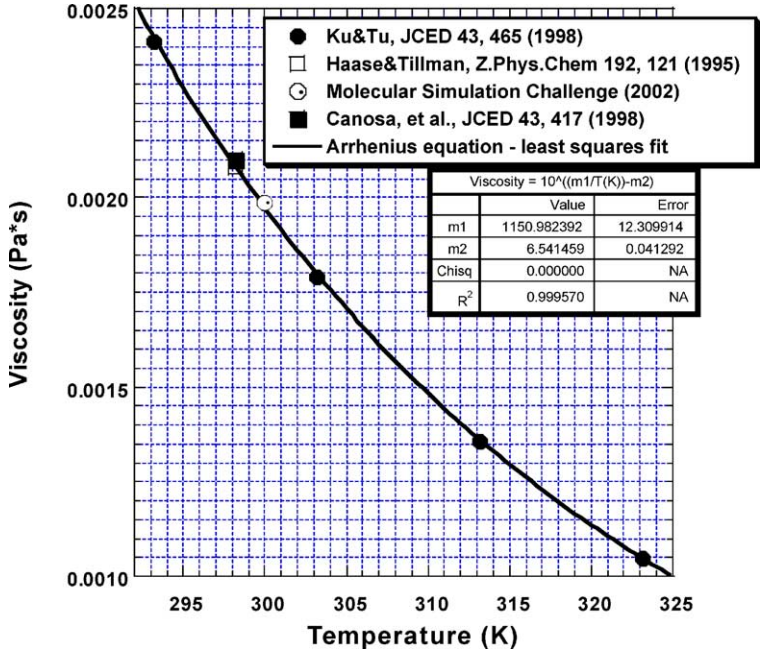

Fig. 1. Viscosity vs. temperature data for 2-propanol. Data are from the literature (references imbedded) and from experiments performed for this problem.

[8–10]. The rms error for the fit is 0.53% and the derived value at 300 K is 1.973 mPa s, 0.76% lower than the comparable contest value of 1.986 mPa s.

Watts and Louie [11] have shown that the uncertainty of density measurements using vibrating-tube densimeters is greater than the precision of replicate experiments. Their work suggests that typical liquid density uncertainties are on the order of 0.17 kg m^{-3}. This margin is similar to that given by Fitzgerald [12] for typical vibrating-tube densimeters that were calibrated according to the manufacturer's instructions, 0.15 kg m^{-3}.

The uncertainties of the contest values are larger than the precision rms error uncertainties based on the uncertainty recommendations in ASTM D 445 and on the comparisons to the literature values discussed above. These estimated uncertainties are: 0.007 mPa·s, 0.021 mPa s, 0.008 mPa s and 0.011 mPa s for parts (a), (b), (c), and (d) of the problem, respectively.

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