

Density, Refractive Index, Apparent Specific Volume, and Electrical Conductivity of Aqueous Solutions of Poly(ethylene glycol) 1500 at Different Temperatures

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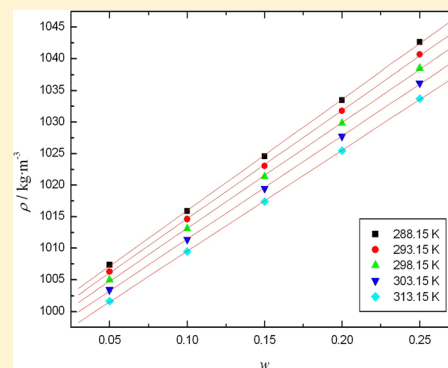
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ABSTRACT: Thermophysical properties of aqueous solutions of poly(ethylene glycol) 1500 g·mol⁻¹ were measured as a function of polymer concentration $w = (0.05, 0.10, 0.15, 0.20 \text{ and } 0.25)$ and temperature $T/K = (288, 293, 298, 303 \text{ and } 308)$. Aqueous systems composed of poly(ethylene glycol) are frequently used in processes involving the separation of biological compounds. The density of the solutions varied from (1001.68 to 1042.65) kg·m⁻³, the refractive index ranged from (1.3377 to 1.3681), the apparent specific volume was between (0.8336 and 0.8528) g·cm⁻³, and the electrical conductivity varied between (66.22 and 170.29) 10⁻³ mS·cm⁻¹. Polynomial models for the properties as a function of temperature and poly(ethylene glycol) 1500 g·mol⁻¹ concentration were fitted to the experimental data. Models accounting for combined effects between variables are particularly useful in industrial applications in which physical parameters must be promptly and accurately calculated.



1. INTRODUCTION

The synthetic polymer known as poly(ethylene glycol) is frequently used in processes involving the separation, concentration, isolation, and purification of biological compounds.^{1–8} For this reason, accurate prediction of the physicochemical properties of aqueous solutions of poly(ethylene glycol) (PEG) is becoming increasingly important.^{9–14} PEG is a neutral polyether composed of repeating ethylene glycol units and is also referred to as poly(ethylene oxide) (PEO) or the IUPAC name poly(oxyethylene) (POE).¹⁵ The material is approved by the U.S. Food and Drug Administration (FDA) as a food ingredient, is nontoxic, weakly immunogenic, and is efficient in the exclusion of other polymers when present in an aqueous environment.^{16–18}

Extraction systems composed of poly(ethylene glycol) 1500 g·mol⁻¹ (PEG1500), salt, and water are classified as aqueous two-phase systems (ATPS). These systems are widely used in the separation of biomolecules^{19–21} due to their mild conditions and greater selectivity, larger difference in density, lower viscosity, and lower cost than ATPS formed from PEG1500 and other polymers such as dextran or maltodextrin.²² The solute partitioning in ATPS systems is affected by factors such as the nature and size of the biocompound, the structure and chain size of the polymer, type of salt, pH, initial composition of the system,

and temperature. Consequently, information concerning the dynamic behavior of aqueous PEG1500 solutions is required for the design of biotechnological processes in which this polymer is used. Data on thermophysical properties of aqueous solutions containing PEG have been reported in the literature, such as for viscosity,^{7–13,22–31} density,^{7–14,22–30} electrical conductivity,^{25,28} apparent specific volume,³² and refractive index.^{25,28,33} However, less accurate equipment and limited temperature ranges still being used to measure thermophysical properties of ATPS. Therefore, we determined the density, refractive index, apparent specific volume and electrical conductivity of aqueous PEG1500 solutions at several concentrations and temperatures. In addition, viscosity data obtained in previous experiments²³ were used to develop predictive models for the systems.

2. EXPERIMENTAL SECTION

2.1. Materials. Poly(ethylene glycol) [HO-(CH₂-CH₂O)_n-CH₂OH] with an average molar mass of 1500 g·mol⁻¹ (PEG1500) and sodium hydroxide (NaOH; mass purity >0.99) were purchased from Vetec Química Fina (Brazil).

Received: September 6, 2013

Accepted: January 7, 2014

Published: January 13, 2014

Solutions were prepared using double distilled and deionized water (electrical resistivity $\approx 18.2 \text{ M}\Omega\cdot\text{cm}$; Master System P&D Gehaka, Brazil). Table 1 presents the sample information.

Table 1. Sample Information

| chemical name | source | initial mass fraction purity | purification method |
|---------------|------------------------|------------------------------|---------------------|
| PEG1500 | Vetec Quim. Fina Ltda. | 0.98 | none |
| NaOH | Vetec Quim. Fina Ltda. | 0.99 | none |

2.2. Measurements. Binary aqueous solutions were prepared on a mass basis using an analytical balance (Denver Instruments, M-310, USA) with an accuracy of $\pm 0.0001 \text{ g}$. A stock solution of PEG1500 ($w = 0.50$) was adjusted to pH 8.0 (PG 100 pHmeter, Gehaka, Brazil) by dropwise addition of NaOH ($1 \text{ mol}\cdot\text{dm}^{-3}$). This pH value is commonly used in ATPS for separation of biological molecules.^{19–22} Appropriate amounts of the stock solution were diluted in 200 cm^3 amber glass bottles and manually stirred to obtain the desired concentrations $w = (0.05, 0.10, 0.15, 0.20, \text{ and } 0.25)$ of PEG1500 aqueous solutions. Densities (ρ) and refractive indexes (n) were measured using a vibrating tube densitometer (DMA4500 Anton Paar, Graz, Austria) and digital refractometer (Abbemat RXA170 Anton Paar, Graz, Austria) thermostatically controlled to $\pm 0.001 \text{ K}$. Both instruments were connected to an automatic sample changer (Xsample 122 Anton Paar, Graz, Austria). Double

distilled and deionized water, and dry air were used as reference substances to calibrate the instruments at atmospheric pressure. The precision of the densitometer was $\pm 1.0\cdot 10^{-5} \text{ g}\cdot\text{cm}^{-3}$ and the precision of the refractometer was $\pm 4.0\cdot 10^{-5}$. The reported results are the average values of three independent measurements for each solution at each of the measurement temperatures $T/\text{K} = (288, 293, 298, 303, \text{ and } 308)$. Electrical conductivities (κ) were determined using a conductivity meter (W12D Bel Engineering, Italy), with an uncertainty of $\pm 0.038 \text{ mS}\cdot\text{cm}^{-1}$. The equipment was calibrated against a KCl solution ($0.01 \text{ mol}\cdot\text{dm}^{-3}$). The cell temperature was controlled using a thermostatic water bath (Q214M2, Quimis Aparelhos Científicos, Brazil). The apparent specific volume ($v_{2\phi}$) was calculated from the density data using eq 1:²⁴

$$v_{2\phi} = \frac{1}{\rho} \left[1 + \frac{\rho_0 - \rho}{w\rho_0} \right] \quad (1)$$

in which $\rho/\text{kg}\cdot\text{m}^{-3}$ and $\rho_0/\text{kg}\cdot\text{m}^{-3}$ are the densities of the polymeric solution and pure water.

2.3. Analysis. All statistical analyses were performed using the Statistical Analysis System version 9.2 software package (SAS Institute Inc., Cary, NC). An analysis of variance (ANOVA) was performed on the models and the model significance was examined using Fisher's statistical test (F -test) to determine significant differences between sources of variation in the experimental results, including the significance of the regression, the lack of fit, and the multiple determination coefficients (R^2).

Table 2. Density ρ , Refractive Index n , Electrical Conductivity κ , and Apparent Specific Volume $v_{2\phi}$ for PEG1500 Aqueous Solutions (w) from $T/\text{K} = (288 \text{ to } 308)^a$

| T K | w | ρ | | n | κ $10^{-3} \text{ mS}\cdot\text{cm}^{-1}$ | $v_{2\phi}$ $\text{g}\cdot\text{cm}^{-3}$ |
|----------|------|-------------------------------|--|---------------------|---|--|
| | | $\text{kg}\cdot\text{m}^{-3}$ | | | | |
| 288 | 0.05 | 1007.39 \pm 0.04 | | 1.3402 \pm 0.0003 | 66.22 \pm 0.32 | 0.8361 \pm 0.0008 |
| | 0.10 | 1015.88 \pm 0.03 | | 1.3469 \pm 0.0001 | 100.99 \pm 0.68 | 0.8356 \pm 0.0003 |
| | 0.15 | 1024.56 \pm 0.05 | | 1.3538 \pm 0.0001 | 123.63 \pm 0.33 | 0.8351 \pm 0.0003 |
| | 0.20 | 1033.49 \pm 0.14 | | 1.3609 \pm 0.0001 | 135.12 \pm 0.48 | 0.8344 \pm 0.0007 |
| | 0.25 | 1042.65 \pm 0.05 | | 1.3681 \pm 0.0001 | 135.99 \pm 0.66 | 0.8336 \pm 0.0002 |
| 293 | 0.05 | 1014.60 \pm 0.02 | | 1.3397 \pm 0.0001 | 68.81 \pm 0.95 | 0.8399 \pm 0.0002 |
| | 0.10 | 1023.06 \pm 0.05 | | 1.3462 \pm 0.0001 | 106.69 \pm 0.20 | 0.8395 \pm 0.0003 |
| | 0.15 | 1031.76 \pm 0.14 | | 1.3531 \pm 0.0001 | 133.40 \pm 0.84 | 0.8389 \pm 0.0007 |
| | 0.20 | 1040.67 \pm 0.06 | | 1.3601 \pm 0.0001 | 146.34 \pm 0.97 | 0.8383 \pm 0.0002 |
| | 0.25 | 1006.31 \pm 0.04 | | 1.3672 \pm 0.0001 | 150.35 \pm 0.09 | 0.8405 \pm 0.0008 |
| 298 | 0.05 | 1013.10 \pm 0.02 | | 1.3391 \pm 0.0002 | 73.61 \pm 1.39 | 0.8441 \pm 0.0002 |
| | 0.10 | 1021.35 \pm 0.06 | | 1.3455 \pm 0.0001 | 112.80 \pm 0.82 | 0.8438 \pm 0.0004 |
| | 0.15 | 1029.83 \pm 0.14 | | 1.3524 \pm 0.0001 | 139.24 \pm 0.26 | 0.8433 \pm 0.0007 |
| | 0.20 | 1038.51 \pm 0.05 | | 1.3593 \pm 0.0001 | 154.01 \pm 0.40 | 0.8428 \pm 0.0002 |
| | 0.25 | 1004.99 \pm 0.04 | | 1.3663 \pm 0.0001 | 158.33 \pm 0.24 | 0.8445 \pm 0.0008 |
| 303 | 0.05 | 1011.38 \pm 0.02 | | 1.3384 \pm 0.0002 | 72.99 \pm 0.69 | 0.8482 \pm 0.0002 |
| | 0.10 | 1019.45 \pm 0.06 | | 1.3448 \pm 0.0001 | 113.90 \pm 0.45 | 0.8480 \pm 0.0004 |
| | 0.15 | 1027.73 \pm 0.14 | | 1.3515 \pm 0.0001 | 141.93 \pm 0.17 | 0.8476 \pm 0.0007 |
| | 0.20 | 1036.19 \pm 0.07 | | 1.3584 \pm 0.0001 | 157.27 \pm 0.99 | 0.8472 \pm 0.0002 |
| | 0.25 | 1003.43 \pm 0.03 | | 1.3653 \pm 0.0001 | 163.17 \pm 1.01 | 0.8485 \pm 0.0007 |
| 308 | 0.05 | 1001.68 \pm 0.04 | | 1.3377 \pm 0.0002 | 73.60 \pm 0.86 | 0.8528 \pm 0.0008 |
| | 0.10 | 1009.46 \pm 0.01 | | 1.3440 \pm 0.0001 | 114.87 \pm 0.55 | 0.8524 \pm 0.0001 |
| | 0.15 | 1017.37 \pm 0.06 | | 1.3507 \pm 0.0001 | 143.09 \pm 0.36 | 0.8522 \pm 0.0004 |
| | 0.20 | 1025.47 \pm 0.14 | | 1.3575 \pm 0.0001 | 160.39 \pm 0.53 | 0.8519 \pm 0.0006 |
| | 0.25 | 1033.74 \pm 0.04 | | 1.3643 \pm 0.0001 | 170.28 \pm 6.20 | 0.8515 \pm 0.0002 |

^aFor densities and refractive index the standard uncertainties u are $u(T) = 0.001 \text{ K}$ and expanded uncertainties are $U(w) = 0.005$; $U(\rho) = 0.2 \text{ kg}\cdot\text{m}^{-3}$; $U(n) = 0.001$ and $U(v_{2\phi}) = 0.002 \text{ g}\cdot\text{cm}^{-3}$. For electrical conductivity the standard uncertainties u are $u(T) = 0.2 \text{ K}$; and expanded uncertainties are $U(\kappa) = 0.002 \text{ mS}\cdot\text{cm}^{-1}$.

The correlation coefficients between the predicted and observed values were calculated for all of the models. The expanded uncertainties in density, refractive index, apparent specific volume, electrical conductivity, and viscosity were calculated as combined uncertainties multiplied by 2. The coverage factor of 2 yields a 95% confidence interval.

3. RESULTS AND DISCUSSION

The density, refractive index, apparent specific volume, and electrical conductivity of the PEG1500 solutions were measured at different temperatures $T/K = (288, 293, 298, 303 \text{ and } 308)$ and the viscosity was previously measured²³ at temperatures $T/K = (283, 288, 293, 298 \text{ and } 303)$. The PEG concentration was $w = (0.05, 0.10, 0.15, 0.20, \text{ and } 0.25)$ by mass. This combination of parameters provided a minimum of 96 experimental values, including independent repetitions, for each property. Table 2 contains the density, refractive index, apparent specific volume, and electrical conductivity measurements, and Table 3 contains the viscosity measurements.²³ Figures 1 to 5 illustrate the behavior of the various properties as a function of PEG1500 concentration and temperature.

Table 3. Viscosity η of Aqueous Binary Solutions of PEG1500 (w) from $T/K = (283 \text{ to } 303)^b$

| T/K | w | $\eta/\text{mPa}\cdot\text{s}$ |
|-------|------|--------------------------------|
| 283 | 0.05 | 1.837 ± 0.084 |
| | 0.10 | 2.771 ± 0.094 |
| | 0.15 | 4.210 ± 0.079 |
| | 0.20 | 6.216 ± 0.153 |
| | 0.25 | 9.173 ± 0.229 |
| 288 | 0.05 | 1.573 ± 0.050 |
| | 0.10 | 2.335 ± 0.050 |
| | 0.15 | 3.481 ± 0.247 |
| | 0.20 | 5.115 ± 0.261 |
| | 0.25 | 7.572 ± 0.501 |
| 293 | 0.05 | 1.443 ± 0.081 |
| | 0.10 | 2.090 ± 0.055 |
| | 0.15 | 3.157 ± 0.071 |
| | 0.20 | 4.537 ± 0.085 |
| | 0.25 | 6.637 ± 0.111 |
| 298 | 0.05 | 1.293 ± 0.061 |
| | 0.10 | 1.860 ± 0.053 |
| | 0.15 | 2.786 ± 0.014 |
| | 0.20 | 4.026 ± 0.040 |
| | 0.25 | 5.743 ± 0.040 |
| 303 | 0.05 | 1.172 ± 0.020 |
| | 0.10 | 1.638 ± 0.078 |
| | 0.15 | 2.414 ± 0.046 |
| | 0.20 | 3.466 ± 0.104 |
| | 0.25 | 4.918 ± 0.099 |

^bThe standard uncertainties u are $u(T) = 0.01 \text{ K}$ and expanded uncertainties are $U(w) = 0.005$ and $U(\eta) = 0.1 \text{ mPa}\cdot\text{s}$.

3.1. Density, Refractive Index, and Apparent Specific Volume. Figure 1 is a plot of density as a function of temperature and concentration. The density of the solutions varied from $(1001.68 \text{ to } 1042.65) \text{ kg}\cdot\text{m}^{-3}$, the refractive index ranged from $(1.3377 \text{ to } 1.3681)$, and the apparent specific volume was between $(0.8336 \text{ and } 0.8528) \text{ g}\cdot\text{cm}^{-3}$. The density increased with increasing PEG1500 concentration and decreased with increasing temperature for constant PEG1500 composition. Similar behavior may be observed in Figure 2 for the refractive index

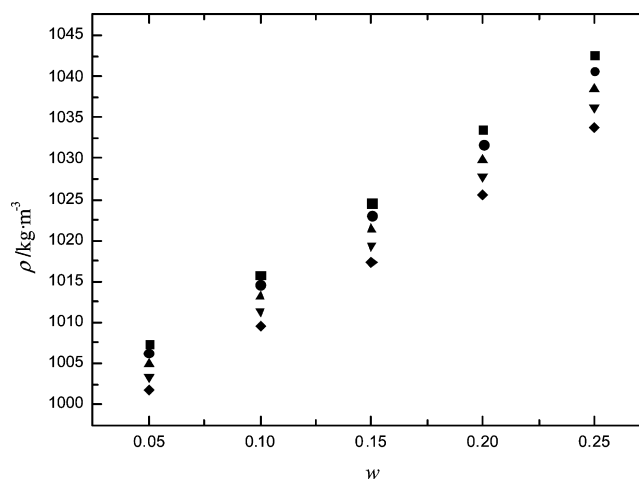


Figure 1. Density ρ of aqueous solutions of PEG1500 as function of mass fraction at different temperatures, T/K : ■, 288; ●, 293; ▲, 298; ▼, 303; ◆, 308.

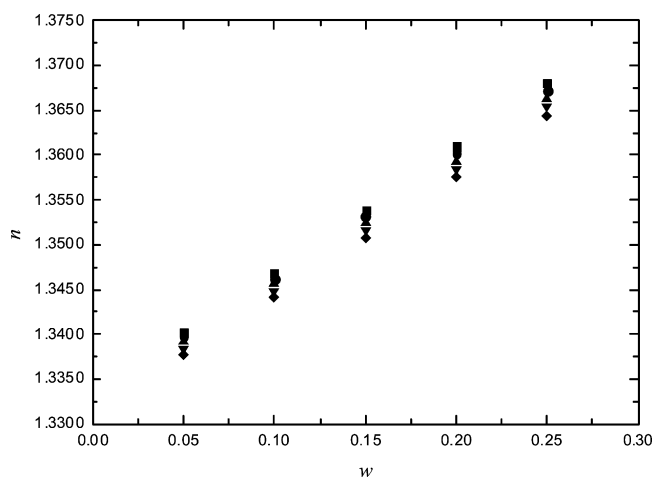


Figure 2. Refractive index n of aqueous solutions of PEG1500 as function of mass fraction at different temperatures, T/K : ■, 288; ●, 293; ▲, 298; ▼, 303; ◆, 308.

under the same conditions of PEG1500 composition and temperature. The apparent specific volume ($v_{2\phi}$) decreased with both increasing polymer concentration and increasing temperature (Figure 3 and Table 2). Density, refractive index, and apparent specific volume all varied linearly with PEG1500 mass fraction (w) under the studied conditions and could be estimated using the general linear model in eq 2:

$$\psi = a_1 + a_2 w \quad (2)$$

where ψ is the physical property and a_1 and a_2 are constants derived from the experimental data. Table 4 contains the coefficients obtained from regression analyses of density, refractive index, and apparent specific volume, the determination coefficients, and the correlation coefficients between the observed and predicted values. The agreement between the experimental and predicted values for density, refractive index and apparent specific volume was very good, with determination coefficients (R^2) for density and refractive index exceeding 0.99 in all cases and determination coefficients for apparent specific volume exceeding 0.97. In all cases the correlation coefficient between the observed and predicted values exceeded 0.99. The densities of the PEG solutions were similar to those reported by

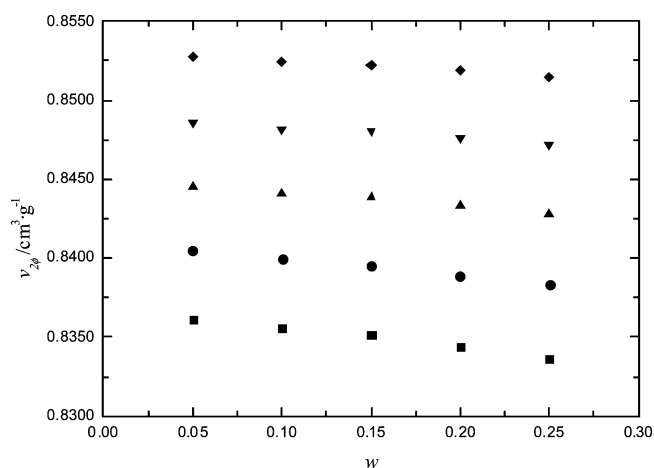


Figure 3. Apparent specific volume v_{20} of aqueous solutions of PEG1500 as function of mass fraction at different temperatures, T/K : ■, 288; ●, 293; ▲, 298; ▼, 303; ◆, 308.

Table 4. Adjusted Parameters of Linear Model for Density (ρ), Refractive Index (n) and Apparent Specific Volume (v_{20}) as Functions of Mass Fraction (w) for PEG1500 Aqueous Solutions between 288 and 308 K

| T/K | α_1 | α_2 | R^2 | correlation coefficient |
|-------|--------------------------------------|------------|--------|-------------------------|
| | $\rho / \text{kg}\cdot\text{m}^{-3}$ | | | |
| 288 | 998.35 | 176.28 | 0.9997 | 0.9998 |
| 293 | 997.51 | 171.74 | 0.9997 | 0.9998 |
| 298 | 996.42 | 167.56 | 0.9997 | 0.9998 |
| 303 | 995.08 | 163.72 | 0.9998 | 0.9999 |
| 308 | 993.50 | 160.26 | 0.9998 | 0.9999 |
| | n | | | |
| 288 | 1.3330 | 0.1396 | 0.9997 | 0.9993 |
| 293 | 1.3326 | 0.1378 | 0.9996 | 0.9998 |
| 298 | 1.3320 | 0.1362 | 0.9996 | 0.9998 |
| 303 | 1.3315 | 0.1347 | 0.9996 | 0.9998 |
| 308 | 1.3308 | 0.1333 | 0.9996 | 0.9998 |
| | $v_{20}/\text{g}\cdot\text{cm}^{-3}$ | | | |
| 288 | 0.8368 | -0.1250 | 0.9931 | 0.9965 |
| 293 | 0.8411 | -0.0109 | 0.9941 | 0.9965 |
| 298 | 0.8450 | -0.0085 | 0.9856 | 0.9971 |
| 303 | 0.8489 | -0.0065 | 0.9779 | 0.9971 |
| 308 | 0.8531 | -0.0062 | 0.9880 | 0.9927 |

Mohsen-Nia et al.,²⁵ who obtained density values ranging from (997.8 to 1025.0) $\text{kg}\cdot\text{m}^{-3}$ for PEG1000 and (998.4 to 1027.8) $\text{kg}\cdot\text{m}^{-3}$ for PEG10000.

3.2. Viscosity. The viscosity of aqueous PEG1500 solutions, previously obtained using a cone and plate sensor,²³ increased with increasing polymer concentration and decreased with increasing temperature (Figure 4). The viscosity ranged from (1.172 to 9.173) mPa·s. To analyze the influence of temperature on viscosity the general quadratic model (eq 3) was employed. Table 5 contains the coefficients obtained from the polynomial regression for viscosity.

$$\psi = a'_1 + a'_2 w + a'_3 w^2 \quad (3)$$

The parameters a'_1 , a'_2 , and a'_3 are constants obtained from the experimental data. Cruz et al.²⁶ measured the viscosities of PEG1500 solutions at temperatures from (318.15 to 363.15) K using glass capillary viscometers. Telis-Romero et al.²⁷ obtained viscosities for PEG1500 solutions with concentrations ranging

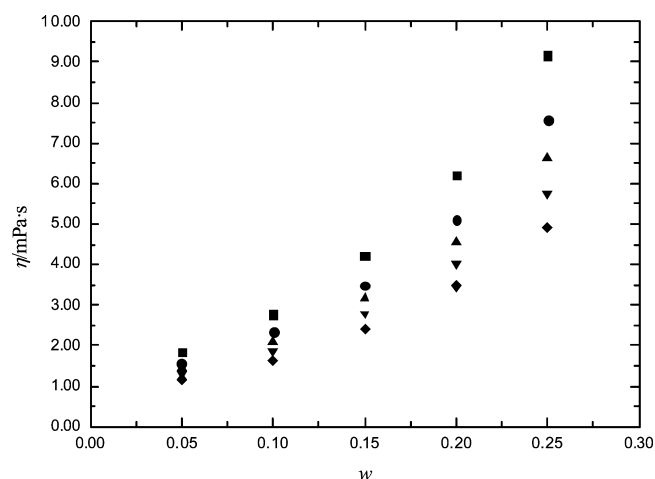


Figure 4. Viscosity η of aqueous solutions of PEG1500 as function of mass fraction at different temperatures, T/K : ■, 283; ●, 288; ▲, 293; ▼, 298; ◆, 303.

Table 5. Adjusted Parameters for Quadratic Model of Viscosity (η) and Electrical Conductivity (κ) as Function of Mass Fraction (w) for PEG1500 Aqueous Solutions at Temperatures $T/K = (283 \text{ to } 303)$ for Viscosity and $T/K = (288 \text{ to } 308)$ for Electrical Conductivity

| T/K | a'_1 | a'_2 | a'_3 | R^2 | correlation coefficient |
|-------|--|----------|-----------|--------|-------------------------|
| | $\eta/\text{mPa}\cdot\text{s}$ | | | | |
| 283 | 1.712 | -3.294 | 131.761 | 0.9974 | 0.9987 |
| 288 | 1.521 | -3.876 | 111.629 | 0.9876 | 0.9938 |
| 293 | 1.331 | -1.920 | 91.961 | 0.9979 | 0.9989 |
| 298 | 1.129 | -0.277 | 74.695 | 0.9993 | 0.9803 |
| 303 | 1.049 | -0.621 | 64.209 | 0.9977 | 0.9996 |
| | $\kappa/10^{-3} \text{ mS}\cdot\text{cm}^{-1}$ | | | | |
| 288 | 20.813 | 1024.095 | -2255.873 | 0.9996 | 0.9996 |
| 293 | 19.546 | 1104.060 | -2328.57 | 0.9993 | 0.9997 |
| 298 | 23.697 | 1119.120 | -2326.03 | 0.9995 | 0.9997 |
| 303 | 21.373 | 1156.492 | -2363.492 | 0.9994 | 0.9997 |
| 308 | 23.942 | 1109.279 | -2105.079 | 0.9951 | 0.9975 |

from (0.10 to 0.22) mass fraction at 303.15 K and pH 7 using a concentric cylinder rheometer. These authors also found a nonlinear correlation between viscosity and PEG1500 concentration. Mohsen-Nia et al.²⁵ studied aqueous mixtures of PEG1000 and PEG10000 at temperatures from (298.15 to 328.15) K and PEG concentrations ranging from $w = (0.05 \text{ to } 0.15)$. The viscosities ranged from (0.509 to 2.270) mPa·s for PEG1000 and were approximately 20% higher for PEG10000.

3.3. Electrical Conductivity. Figure 5 depicts the electrical conductivity (κ) of aqueous solutions of PEG1500 as a function of mass fraction and temperature. The conductivity increased with increasing temperature and polymer concentration. The electrical conductivity varied between (66.22 and 170.29) $10^{-3} \text{ mS}\cdot\text{cm}^{-1}$. The influence of temperature on κ was modeled using the general quadratic model in eq 3. The coefficients obtained from the polynomial regression, the R^2 values, and the correlation coefficients between the observed and predicted values are listed in Table 5. Silva et al.²⁸ studied the thermophysical properties of aqueous PEG4000 mixtures at temperatures between (278.15 and 318.15) K. The electrical conductivities ranged from (28 to 140) $10^{-3} \text{ mS}\cdot\text{cm}^{-1}$.

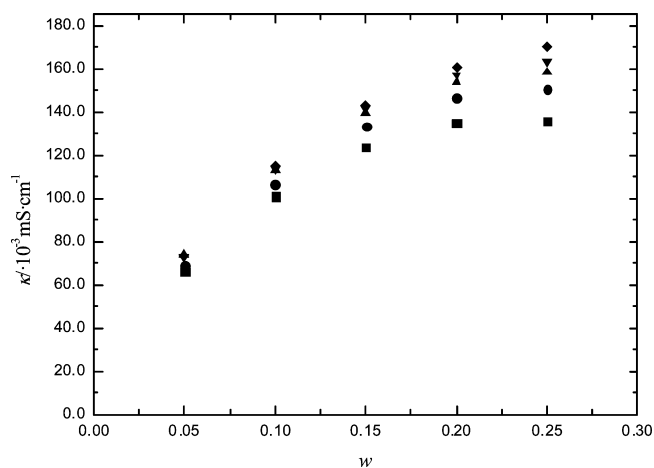


Figure 5. Electrical conductivity κ of aqueous solutions of PEG 1500 as function of mass fraction at different temperatures, T/K : ■, 288; ●, 293; ▲, 298; ▼, 303; ◆, 308.

3.4. Combined Effect of Temperature and Concentration. Polynomial models of thermophysical properties as a function of temperature and PEG1500 concentration were constructed by fitting the experimental data to the general quadratic model in eq 4. Nonsignificant parameters were eliminated on the basis of Student's t -test and p values less than 0.05.

$$\psi = \beta_1 + \beta_2 w + \beta_3 T + \beta_4 w^2 + \beta_5 T^2 + \beta_6 wT \quad (4)$$

ψ is the thermophysical property and $\beta_1, \beta_2, \beta_3, \beta_4, \beta_5,$ and β_6 are constants determined from the experimental data. Table 6 contains the coefficients obtained from the polynomial regression for the predictive models based on the master model (eq 4) for density (ρ), refractive index (n), viscosity (η), electrical conductivity (κ), and apparent specific volume ($v_{2\theta}$). The agreement between the experimental and predicted values for thermophysical properties was good, with all R^2 values and correlation coefficients greater than 0.99.

Lee and Teja²⁹ analyzed the influence of temperature on viscosity, and we employed their proposed equation in our research (eq 5):

$$\ln(\eta) = A + \frac{B}{T - C} \quad (5)$$

In this equation $A, B,$ and C are the model parameters and T/K . The values of $A, B,$ and C were obtained through nonlinear regression analysis of eq 5 (Table 7). González-Tello et al.³⁰ described the influence of PEG concentration on the B parameter when analyzing the combined effect of temperature and polymer concentration on viscosity. Among the relations they tested, the optimum model was linear. Even so, the best correlation was achieved for solutions with values of $\eta \geq 10$ mPa·s. Subsequently,

Table 7. Adjusted Parameters for Lee and Teja²⁸ Model (eq 5) of Viscosity (η) as Function of Temperature for PEG1500 Aqueous Solutions from $w = (0.05 \text{ to } 0.25)$ ²³

| w | A | B | C | R^2 | correlation coefficient |
|------|---------|----------|----------|--------|-------------------------|
| 0.05 | -1.3400 | 133.0061 | 214.6703 | 0.9958 | 0.9999 |
| 0.10 | -1.7813 | 249.0570 | 194.0110 | 0.9969 | 0.9999 |
| 0.15 | -2.0597 | 385.1332 | 172.6764 | 0.9921 | 0.9999 |
| 0.20 | -2.4495 | 559.0140 | 152.0191 | 0.9943 | 0.9999 |
| 0.25 | -3.0383 | 798.5563 | 130.9669 | 0.9976 | 0.9999 |

researchers have used the González-Tello et al.³⁰ equation (eq 6) to correlate the dynamic viscosity of several binary aqueous polymer mixtures.

$$\ln(\eta) = P1 + \frac{(P2 + P3w)}{T - P4} \quad (6)$$

Figure 6 illustrates the influence of PEG1500 concentration on the parameter B in solutions with mass fractions w from (0.05 to

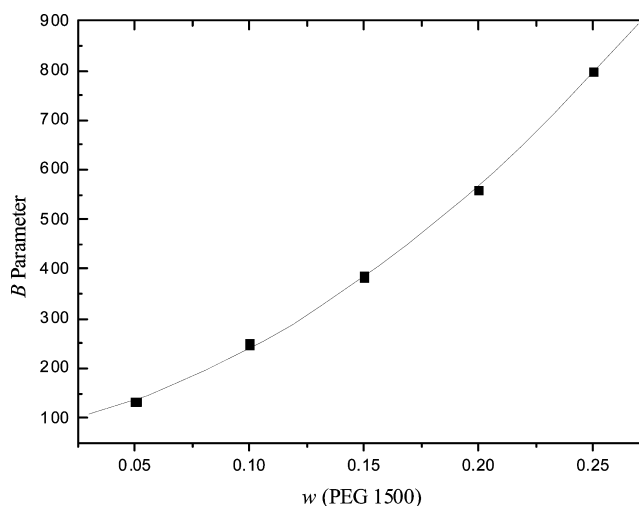


Figure 6. Variation of B parameter (eq 5) with PEG 1500 mass fraction (w); ■, quadratic model.

0.25). A quadratic model provided the best fit to the experimental data using the coefficients in eq 7:

$$B = 75.0266 + 841.1170w + 8136.6840w^2 \quad (7)$$

Combining the quadratic model of eq 3 for B with eq 5 to represent the influence of temperature and concentration on viscosity yields eq 8:

$$\ln(\eta) = P1 + \frac{(P2 + P3w + P4w^2)}{T - P5} \quad (8)$$

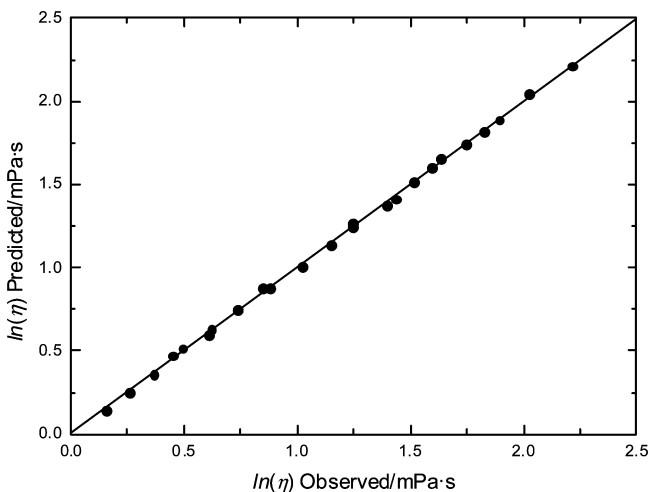
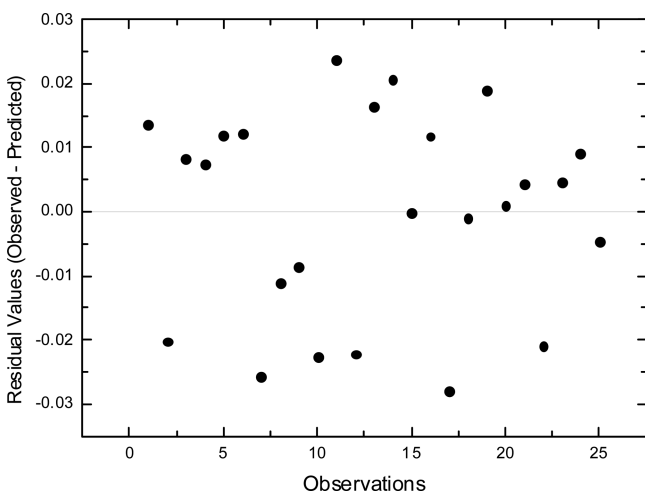
Table 6. Adjusted Parameters for Master Model (eq 4) for Density (ρ), Refractive Index (n), Viscosity (η), Electrical Conductivity (κ), and Apparent Specific Volume ($v_{2\theta}$) of Aqueous PEG1500 Solutions

| properties | β_1 | β_2 | β_3 | β_4 | β_5 | β_6 | R^2 | correlation coefficient |
|--|-----------|-----------|-----------|-----------|-----------|-----------|--------|-------------------------|
| $\rho/\text{kg}\cdot\text{m}^{-3}$ | 1000.69 | 176.29 | -0.05 | 38.87 | -0.00 | -0.80 | 0.9999 | 0.9999 |
| n | 1.3347 | 0.1348 | 0.0000 | 0.0311 | 0.0000 | -0.0031 | 0.9998 | 0.9999 |
| $\eta/\text{mPa}\cdot\text{s}$ | 195.909 | 247.847 | -1.354 | 94.681 | -0.002 | -0.852 | 0.9920 | 0.9960 |
| $\kappa/10^{-3} \text{ mS}\cdot\text{cm}^{-1}$ | -3454.18 | 496.98 | -23.18 | 2247.36 | -0.00 | 5.31 | 0.9972 | 0.9986 |
| $v_{2\theta}/\text{g}\cdot\text{cm}^{-3}$ | 0.8238 | -0.1413 | 0.0008 | -0.0107 | 0.0000 | 0.0003 | 0.9998 | 0.9999 |

Table 8. Adjusted Parameters for Model Described by eq 7 for Viscosity (η) as Function of Temperature and Mass Fraction for PEG1500 Aqueous Solutions.²³

| P1 | P2 | P3 | P4 | P5 | R ² | correlation coefficient |
|----------|----------|-----------|-----------|----------|----------------|-------------------------|
| -3.76406 | 687.9860 | 1466.7646 | -183.9292 | 108.5837 | 0.9992 | 0.9996 |

where P1, P2, P3, P4, and P5 are the model parameters derived from the experimental data. The values presented in Table 8 were determined using nonlinear regression. In our research $\eta < 10$ mPa·s for all samples. Figures 7 and 8 are plots of the residuals

**Figure 7.** Predicted (eq 7) versus observed values of viscosity in PEG1500 solutions for $T/K = (283 \text{ to } 303)$ and $w = (0.05 \text{ to } 0.25)$.**Figure 8.** Residuals for viscosity (observed – predicted (eq 7)) versus observations in PEG1500 solutions for $T/K = (283 \text{ to } 303)$ and $w = (0.05 \text{ to } 0.25)$.

and predicted versus observed values for this model. The straight 45° slope of Figure 8 indicates no significant deviation between the calculated and observed values and confirms the robustness of the model in predicting the properties of PEG1500 solutions.

4. CONCLUSIONS

Thermophysical properties density (ρ), refractive index (n), viscosity (η), electrical conductivity (κ), and apparent specific volume ($v_{2\phi}$) were measured for aqueous solutions of poly(ethylene glycol) 1500 g·mol⁻¹ at different temperatures.

Polynomial models for the properties were well adjusted to the experimental data.

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Funding

We are thankful to the Brazilian agencies CAPES, CNPq, FAPEMIG, and FAPESP for the financial support, fellowships, and grants.

Notes

The authors declare no competing financial interest.

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