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Mathematical modeling of glycerol aqueous solutions thermophysical properties. Case study of density and viscosity

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Abstract

Purified glycerol resulted from various processes is mixed with water in different proportions and successfully employed in food industry as humectant, solvent, sweetener, preservative agent etc. Thermophysical properties of glycerol aqueous solutions are needed to determine information required to design and optimize the industrial equipment. Through this paper several mathematical connections were established between density and viscosity of glycerol aqueous solutions and two main parameters influencing their behavior: temperature and concentration. For both mentioned properties concentration varied from 0 to 100%. For temperature, ranges between 288.15 and 303.15 K for density and between 233.15 and 373.15 K for dynamic viscosity were considered. The regressions analysis conducted indicated no statistical differences between existing data and those obtained with developed models. This fact is sustained also by the values registered for the correlation coefficient which were higher than 0.96 for all the resulted equations suggesting a good fit with published data.

Keywords: glycerol, density, viscosity, thermophysical properties, mathematical modeling

1. Introduction

Glycerol is a sweet-tasting, colorless, odorless, viscous, hygroscopic trihydric sugar alcohol miscible with water and ethanol [1]. It can be obtained through different processes such as microbial fermentation [2,3], industrial conversion of lignocelluloses into ethanol [4-6], soap or biodiesel manufacture etc. [7,8]. In the last mentioned process for example it is a major by-product representing approximately 10% reported at the amount of the main product. Since it was projected that by 2016 more than 15 billion liters of crude glycerol would be produced worldwide, the development of sustainable processes utilizing this organic raw material is highly recommended [9]. The unique combination of its physical and chemical properties makes glycerol a versatile product, readily compatible with many other substances and easy to handle. Glycerol is also virtually nontoxic to human health and to environment. Therefore, after an attentive purification [10], it can be a useful material in various areas of application [11-13] one of them being represented by the food industry. Glycerol aqueous solutions serve as humectant, solvent, sweetener and preservative agent in the beverages, as filler in biocomposite films production [14], as a thickening agent in liqueurs, as ester in shortenings and margarine [15]. Glycerol is known also as a good emulsifying agent. It can alter the magnitude of the repulsive and attractive forces governing the stability and rheological properties of an emulsion influencing its stability, rheological and optical properties [16]. Glycerol has been also used as texturizer, as plasticizer [17], as softening agent in bread [18],

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cakes [19], cheese and candy [20], as hypertonic media for meat foodstuffs [16] etc.

Thermophysical properties of glycerol aqueous solutions are fundamental variables that need to be considered for the design of industrial equipment employed in food industry. Properties such as density and viscosity are needed to determine behavioral and predictive information to optimize the involved unit operations. The present work was motivated by the fact that even though there are data on density and viscosity of glycerol-water mixtures [21,22], they are often found as tabular or graphical representations which are not appropriate for a proper use. Therefore, the specific objective of this work was to establish mathematical models suitable for adequate computer software development which can be easily used in the industrial field. As consequence, the dependency of glycerol aqueous solutions on concentration and temperature was studied. The obtained mathematical equations were compared with the existing data by the mean of different statistical analysis in order to establish if they describe accurately the behavior of glycerol-water mixtures thermophysical properties.

2. Materials and methods

Technical and scientific literature [22,23] have provided, for the regression analysis, the data concerning the density (ρ, kg·m^{-3}) (Table 1) and dynamic (η, Pa·s) (Table 2) and kinematic viscosity (ν, m^{2}·s^{-1}) variations of glycerol with concentration ($C_{\%}$, w/w) and temperature (t, °C or T, K).

In order to generate mathematical models able to describe and predict the tendency of the glycerol thermo-physical properties and to analyze them, the following computer software were employed: Microsoft Excel™ 2013, CurveExpert® software, TableCurve 3D® v.4 and XLSTAT-Pro v.7.5. Studied thermophysical properties of glycerol aqueous solutions were represented as functions of temperature and concentration. The adequacy of the resulted mathematical models was tested by the method of least squares, relative error ε in absolute value (Equation 1) and ANOVA.

$$\varepsilon_{\%} = \left| \frac{Data_{experimental} - Data_{calculated}}{Data_{experimental}} \right| \cdot 100\,[\%] \quad \textbf{(1)}$$

3D graphical representation (Figure 1a and 1b) of the existing data of glycerol aqueous solutions density and dynamic viscosity offer an illustrated perspective of the variation with the imposed parameters. These variations, with a single or both state parameters in the same time, can be described by the equation generator of the employed software. As it can be seen from the examples given in equations 2, 3 and 4 with their respective coefficients presented in Table 3, the established correlations are rather complex and difficult to use.

$$\rho = \frac{a + b \cdot C_{\%} + c \cdot C_{\%}^2 + d \cdot C_{\%}^3 + e \cdot T + f \cdot T^2}{1 + g \cdot C_{\%} + h \cdot C_{\%}^2 + i \cdot T} \quad \textbf{(2)}$$

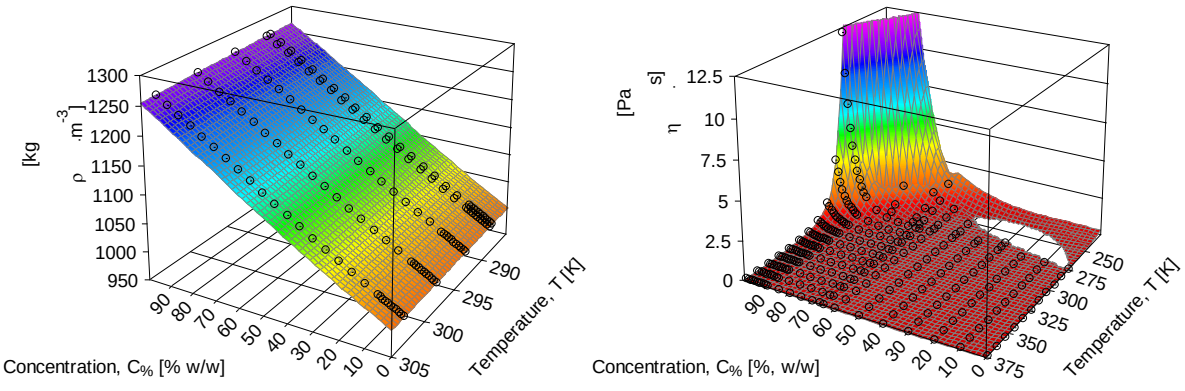
$$\ln(\eta) = a + b \cdot C_{\%} \cdot \ln(C_{\%}) + c \cdot C_{\%}^{1.5} + d \cdot C_{\%}^{2.5} + e \cdot (\ln(T))^2 + f \cdot T^{0.5} + \frac{g}{\ln(T)} + \frac{h}{T^{0.5}} + \frac{i \cdot \ln(T)}{T} \quad \textbf{(3)}$$

$$\ln(\eta) = a + b \cdot C_{\%} + c \cdot C_{\%}^3 + d \cdot \ln(T) + \frac{e}{T^{0.5}} + \frac{f \cdot \ln(T)}{T} \quad \textbf{(4)}$$

Table 1. Glycerol density, (ρ, kg.m-3)

Concentration,	**Temperature, T [K]**				
$C_{\%}$ [% w/w]	**288.15**	**288.65**	**293.15**	**298.15**	**303.15**
100	1264.15	1263.81	1261.08	1258.02	1254.95
95	1251.30	1250.95	1248.25	1245.15	1241.90
90	1238.10	1237.75	1235.10	1232.00	1228.90
85	1224.85	1224.45	1221.80	1218.70	1215.65
80	1211.60	1211.20	1208.50	1205.45	1202.40
75	1197.85	1197.50	1194.85	1191.95	1189.00

70	1184.15	1183.85	1181.25	1178.40	1175.65
65	1170.30	1170.00	1167.50	1164.75	1161.95
60	1156.50	1156.15	1153.80	1151.05	1148.30
55	1142.60	1142.30	1140.05	1137.40	1134.70
50	1128.70	1128.45	1126.30	1123.75	1121.10
45	1115.10	1114.60	1112.80	1110.40	1107.95
40	1101.45	1101.30	1099.30	1097.10	1094.75
35	1088.00	1087.80	1086.00	1083.90	1081.65
30	1074.55	1074.35	1072.70	1070.70	1068.55
25	1061.50	1061.30	1059.80	1058.00	1056.05
20	1048.40	1048.25	1046.90	1045.25	1043.50
15	1035.80	1035.70	1034.50	1033.00	1031.30
10	1023.25	1023.15	1022.10	1020.70	1019.05
9	1020.85	1020.75	1019.70	1018.35	1016.70
8	1018.40	1018.35	1017.30	1016.00	1014.40
7	1016.00	1015.90	1014.95	1013.60	1012.05
6	1013.60	1013.50	1012.55	1011.25	1009.70
5	1011.20	1011.10	1010.15	1008.90	1007.35
4	1008.75	1008.70	1007.80	1006.55	1005.05
3	1006.35	1006.30	1005.40	1004.15	1002.70
2	1003.95	1003.85	1003.00	1001.80	1000.35
1	1001.53	1001.45	1000.60	999.45	998.00
0	999.13	999.05	998.23	997.08	995.68



(a) (b)

Table 2. Phenolic acids, flavones and flavonols of *Glycine max*, *Vigna radiata* and *Medicago sativa* sprouts (mg/kg) [7].

Table 2. Glycerol dynamic viscosity, (η, Pa·s)

Concentration,	Temperature, T [K]															
$C_{\%}$ [% w/w]	233.15	243.15	253.15	263.15	268.15	273.15	283.15	293.15	303.15	313.15	323.15	333.15	343.15	353.15	363.15	373.15
100	-	-	-	-	-	12.0700	3.9000	1.4120	0.6120	0.2840	0.1420	0.0813	0.0506	0.0319	0.0213	0.0148
99	-	-	-	-	-	9.4200	3.0900	1.1500	0.5000	0.2350	0.1220	0.0691	0.0436	0.0278	0.0190	0.0132
98	-	-	-	-	-	7.3700	2.4600	0.9390	0.4090	0.1960	0.1040	0.0598	0.0385	0.0248	0.0170	0.0122
97	-	-	-	-	-	5.7700	1.9500	0.7650	0.3400	0.1660	0.0889	0.0519	0.0336	0.0219	0.0151	0.0109
96	-	-	-	-	-	4.6000	1.5850	0.6240	0.2810	0.1420	0.0778	0.0454	0.0297	0.0196	0.0136	0.0101
95	-	-	-	-	-	3.6900	1.2700	0.5230	0.2370	0.1210	0.0670	0.0399	0.0264	0.0175	0.0124	0.0091
94	-	-	-	-	-	2.9300	1.0400	0.4370	0.2020	0.1050	0.0584	0.0354	0.0236	0.0158	0.0112	0.0082
93	-	-	-	-	-	2.4000	0.8600	0.3670	0.1720	0.0890	0.0515	0.0316	0.0212	0.0144	0.0103	0.0075
92	-	-	-	-	-	1.9500	0.7290	0.3100	0.1470	0.0783	0.0448	0.0280	0.0190	0.0131	0.0095	0.0068
91	-	-	-	-	-	1.5900	0.5920	0.2590	0.1260	0.0681	0.0398	0.0251	0.0171	0.0119	0.0086	0.0064
90	-	-	-	-	-	1.3100	0.4980	0.2190	0.1090	0.0600	0.0355	0.0225	0.0155	0.0110	0.0079	0.0060
85	-	-	-	-	-	0.5400	0.2230	0.1090	0.0580	0.0335	0.0212	0.0142	0.0100	0.0073	0.0055	0.0042
80	-	-	1.6000	0.6830	0.4190	0.2550	0.1160	0.0601	0.0339	0.0208	0.0136	0.0094	0.0069	0.0051	0.0040	0.0032
75	-	-	-	-	-	0.1320	0.0652	0.0355	0.0212	0.0136	0.0093	0.0066	0.0050	0.0038	0.0030	0.0024
70		1.0460	0.3940	0.1510	0.1100	0.0760	0.0388	0.0225	0.0141	0.0094	0.0066	0.0049	0.0038	0.0029	0.0023	0.0019
66.7	1.3980	0.6310	0.2890	0.1130	0.0747	0.0555	0.0269	0.0177	0.0113	0.0077	0.0055	0.0041	0.0032	0.0025	0.0020	0.0017
65	-	-	-	-	-	0.0457	0.0253	0.0152	0.0099	0.0068	0.0049	0.0037	0.0029	0.0023	0.0019	0.0016
60	-	0.2440	0.1080	0.0591	0.0416	0.0299	0.0174	0.0108	0.0072	0.0051	0.0038	0.0029	0.0023	0.0018	0.0015	0.0013
50	-	-	0.0481	0.0244	0.0188	0.0146	0.0090	0.0060	0.0042	0.0031	0.0024	0.0019	0.0015	0.0013	0.0011	0.0009
40	-	-	-		0.0103	0.0083	0.0054	0.0037	0.0027	0.0021	0.0016	0.0013	0.0011	0.0010	0.0008	0.0007
30	-	-	-	0.0144	0.0065	0.0051	0.0035	0.0025	0.0019	0.0015	0.0012	0.0010	0.0008	0.0006	0.0007	0.0006
20	-	-	-	-	-	0.0034	0.0024	0.0018	0.0014	0.0011	0.0009	0.0007	0.0006	0.0006	0.0005	0.0004
10	-	-	-	-	-	0.0024	0.0017	0.0013	0.0010	0.0008	0.0007	0.0006	0.0005	0.0004	0.0004	0.0003
0	-	-	-	-	-	0.0018	0.0013	0.0010	0.0008	0.0007	0.0005	0.0005	0.0004	0.0004	0.0003	0.0003

Table 3. Generated functions coefficients

Coefficient	Equation 2	Equation 3	Equation 4
a	692.6394305	-8.6379E+06	-34738.9874
b	-8.78548851	0.116971892	0.013927491
c	-0.081146873	-0.06591008	7.73933E-06
d	0.000223395	0.000231969	3846.406359
e	4.207930603	63022.15039	356121.654
f	-0.00468518	-21354.1815	-408682.827
g	-0.01240993	5.00271E+07	-
h	0.000104671	-2.6234E+07	-
i	0.001795529	-1.5715E+07	-
R^2	0.9999	0.9994	0.9992
Adj R^2	0.9999	0.9993	0.9992

Table 4. Gaussian function coefficients

Temperature, T [K]	Equation 8 coefficients		
	a	***b***	***c***
288.15	2617.918	757.8544	545.7373
288.65	2663.163	773.1982	551.89
293.15	2904.016	852.5041	583.1003
298.15	3233.737	950.8216	619.6178
303.15	3574.27	1042.911	652.0999

Table 4'. Linear function coefficients

Equation 10 coefficients	Equations 3 and 4 coefficients	
	x	***y***
	Linear model (*LM*)	
a	- 15540	63.003
b	- 4679	18.877
c	- 1486.8	7.0597

For both density and dynamic viscosity of glycerol solutions, the correlation coefficients registered values above 0.999. In terms of error in absolute value, $\varepsilon_{\%}$ was between 0.01- 0.3% for density. In the case of dynamic viscosity for some data $\varepsilon_{\%}$ reached values over 350% (min: -430.21% and max: 99.45%) the equations generated by the employed software fitting only the plotted points ignoring the real variation.

This fact is illustrated also in Figure 2 which shows residuals for the two studied thermophysical properties.

Due to these considerations, another approach was necessary in order to generate mathematical models.

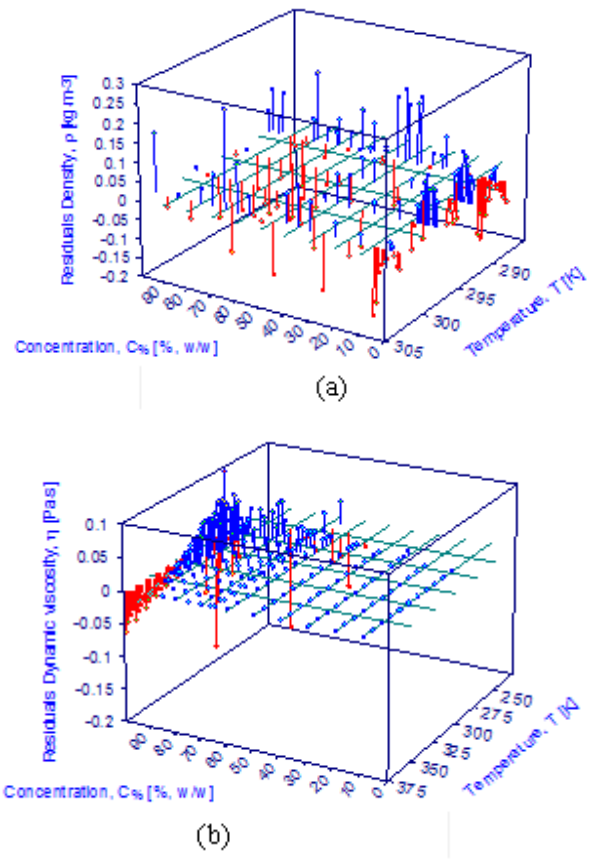


Figure 2. Equation residuals for glycerol density (a) and dynamic viscosity (b)

Density

Using Microsoft Excel™ 2013 spreadsheets and CurveExpert® software, multiple correlations between concentration, $C_{\%}$, [%, w/w], and density, ρ [kg·m^{-3}], at constant temperature T [K] have been established. The equations that fit, with a correlation coefficient over 0.990, all 5 temperature variations were:

polynomial fit of 4th degree:

$$\rho = a + b \cdot C_{\%} + c \cdot C_{\%}^2 + d \cdot C_{\%}^3 + e \cdot C_{\%}^4 \quad \textbf{(5)}$$

Richards model $$\rho = \frac{a}{1 + exp(b - c \cdot C_{\%})^{1/d}} \quad \textbf{(6)}$$

MMF model $$\rho = \frac{a \cdot b + c \cdot C_{\%}^d}{b + C_{\%}^d} \quad \textbf{(7)}$$

Gaussian model $$\rho = a \cdot \exp \frac{-(b - C_{\%})^2}{2 \cdot c^2} \quad \textbf{(8)}$$

logistic model $$\rho = \frac{a}{1 + b \cdot exp(-c \cdot C_{\%})} \quad \textbf{(9)}$$

For this model a Gaussian was chosen. *a*, *b* and *c* coefficients values are presented in *Table 4*.

In order to correlate the coefficients with temperature *T*, [K], different models were used in CurveExpert® software. Considering the best fit and simplicity in formulation a linear model (Equation 10) was selected.

$$LM_{Coefficient} = x + y \cdot T \quad \textbf{(10)}$$

Combining the equations 8 and 10, the final form of the proposed equation model can be expressed by Equation 11. Its regression coefficient R^2 was determined as being 0.9994, fact that confirms that the established mathematical correlation respects the real tendency of thermodynamic properties variation according with state parameters.

$$\rho = LM_a \cdot \exp \frac{-(LM_b - C_{\%})^2}{2 \cdot LM_c^2} \quad \textbf{(5')}$$

Relative error equation was used to compare the values given by the developed model with existing scientific data (Table 1). A final overall average of 0.003% and 1.62% in absolute value was obtained (Table 5). The ANOVA analysis revealed that the sample *P*-value is 0.98749 greater than the targeted alpha 0.05 and the *F crit* value (3.93811) is larger than the *F*-test one (0.000014) indicating that is not a statistical difference between tabular and calculated data.

Table 5. Glycerol density calculated values (C.V.) and the relative errors

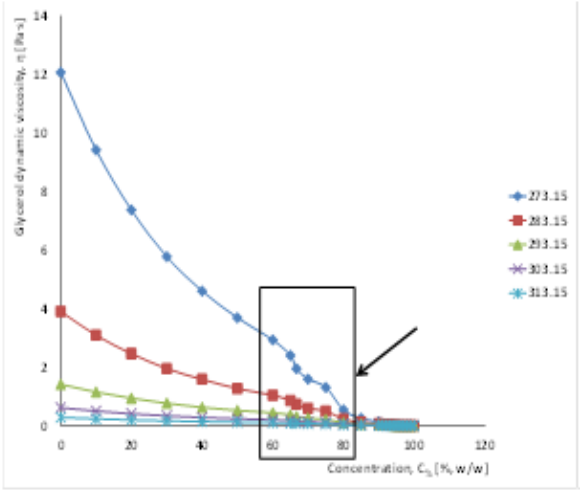
Concentration, $C_{\%}$ [% w/w]	Temperature, T [K]									
	288.15		288.65		293.15		298.15		303.15	
	C. V.	$\varepsilon_{\%}$	C. V.	$\varepsilon_{\%}$	C. V.	$\varepsilon_{\%}$	C. V.	$\varepsilon_{\%}$	C. V.	$\varepsilon_{\%}$
100	1263.0	0.09	1263.8	0.00	1266.3	-0.42	1262.6	-0.36	1254.6	0.02
95	1249.1	0.17	1249.8	0.09	1252.2	-0.32	1248.6	-0.28	1240.8	0.08
90	1235.3	0.22	1236.0	0.14	1238.3	-0.26	1234.6	-0.22	1227.1	0.15
85	1221.5	0.27	1222.2	0.18	1224.3	-0.21	1220.8	-0.17	1213.4	0.18
80	1207.7	0.31	1208.4	0.23	1210.5	-0.17	1207.0	-0.13	1199.8	0.21
75	1194.1	0.31	1194.7	0.23	1196.7	-0.16	1193.3	-0.12	1186.3	0.22
70	1180.4	0.31	1181.1	0.23	1183.0	-0.15	1179.7	-0.11	1172.9	0.23
65	1166.9	0.29	1167.5	0.21	1169.4	-0.17	1166.2	-0.13	1159.6	0.20
60	1153.4	0.27	1154.0	0.19	1155.8	-0.18	1152.7	-0.15	1146.3	0.17
55	1139.9	0.23	1140.5	0.15	1142.3	-0.21	1139.3	-0.17	1133.1	0.13
50	1126.5	0.19	1127.1	0.12	1128.9	-0.24	1126.0	-0.21	1120.1	0.09
45	1113.2	0.16	1113.	0.07	1115	-0.25	1112.8	-0.22	1107.1	0.07
40	1100.0	0.13	1100.5	0.07	1102.3	-0.28	1099.7	-0.24	1094.2	0.05
35	1086.8	0.11	1087.3	0.04	1089.1	-0.29	1086.7	-0.26	1081.3	0.02
30	1073.7	0.08	1074.2	0.01	1076.0	-0.32	1073.7	-0.28	1068.6	-0.01
25	1060.6	0.08	1061.1	0.01	1063.0	-0.31	1060.8	-0.27	1056.0	0.00
20	1047.6	0.07	1048.1	0.01	1050.1	-0.31	1048.0	-0.27	1043.4	0.00
15	1034.7	0.10	1035.2	0.04	1037.2	-0.26	1035.3	-0.23	1031.0	0.03
10	1021.9	0.13	1022.4	0.07	1024.4	-0.23	1022.7	-0.20	1018.6	0.04
9	1019.3	0.14	1019.9	0.08	1021.9	-0.22	1020.2	-0.19	1016.1	0.05
8	1016.8	0.15	1017.3	0.10	1019.3	-0.20	1017.7	-0.17	1013.7	0.07
7	1014.2	0.17	1014.7	0.11	1016.8	-0.18	1015.2	-0.16	1011.2	0.08
6	1011.7	0.18	1012.2	0.12	1014.2	-0.17	1012.7	-0.15	1008.7	0.09
5	1009.1	0.20	1009.7	0.14	1011.7	-0.16	1010.2	-0.13	1006.3	0.10
4	1006.6	0.21	1007.1	0.15	1009.2	-0.14	1007.7	-0.12	1003.8	0.12
3	1004.1	0.22	1004.6	0.17	1006.7	-0.13	1005.2	-0.11	1001.4	0.12
2	1001.5	0.24	1002.0	0.18	1004.1	-0.12	1002.7	-0.09	999.0	0.13
1	999.0	0.25	999.5	0.19	1001.6	-0.11	1000.2	-0.08	996.5	0.14
0	996.5	0.26	997.0	0.20	999.1	-0.09	997.7	-0.07	994.1	0.15

Table 6. Equation 7' coefficients

Equation 6 coefficients	Equation coefficients		
	x	*y*	*z*
Quadratic fit (*QF*)			
Concentration range of 0% to 65%			
a	-77.62961	0.46617324	-0.00050319
b	0.8227745	-0.00560673	7.69E-06
c	0.40758394	-3.8137E-05	4.31E-08
Concentration range of 65% to 90%, temperature 273.15 - 303.15 K			
a	-35.125341	0.24831393	-0.0003818
b	0.33756037	-0.00251914	4.21E-06
c	0.32094168	-0.00081365	1.33E-06
Concentration range of 65% to 90%, temperature 303.15 - 373.15 K			
a	-107.58209	0.60613526	-0.0006527
b	1.122091	-0.00682011	8.62E-06
c	0.50282736	-0.00054874	7.28E-07
Concentration range of 90% to 100%, temperature 273.15 - 323.15 K			
a	14.48131	-0.14007	0.00035746
b	-0.06452	0.000782	-2.29E-06
c	0.409939	-0.00356	9.10E-06
Concentration range of 90% to 100%, temperature 323.15 - 373.15 K			
a	-70.0522	0.329912	-0.0001705
b	0.851722	-0.0046	4.50E-06
c	0.781453	-0.00214	3.01E-06

Dynamic viscosity

In order to develop an accurate mathematical model, with lower relative errors for all calculated data compared with tabular values, than that generated by the employed software, an analysis of the 2D graphical representations of glycerol solutions dynamic viscosity, η [Pa·s], variation with concentration, $C_{\%}$ [%, w/w] at constant temperature, T [K] was necessary. The analysis revealed three different levels of variation for glycerol dynamic viscosity (Figure 3): 0 to 65%, 65% to 90% and respectively 90% to 100%. Even tough, in these conditions, an appropriate description of the above mentioned glycerol thermophysical property variations would be realized by three different correlations, in order to facilitate the use of the developed models, it is recommended to use only an equation type.



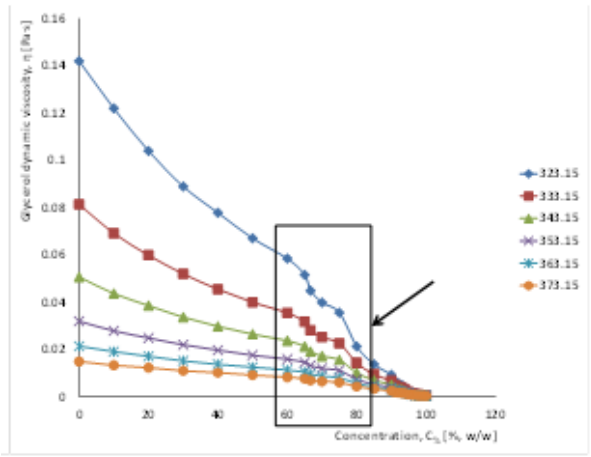


Figure 3. Glycerol dynamic viscosity variation with concentration and temperature

Bleasdale model (Equation 6') was considered adequate to express the connections between concentration, $C_{\%}$, [%, w/w] and dynamic viscosity, η [Pa·s], at constant glycerol temperature *T*, [K]. The correlation coefficient of all equations is over 0.999.

$$\eta = a + b \cdot \ln\left(C_{\%}\right)^{\frac{1}{c}} \quad \textbf{(6')}$$

The *a*, *b* and *c* coefficients values were quadratic fitted with temperature *T*, [K] (Equation 7') for all three chosen ranges, generating the final form of the mathematical model (Equation 8') with the coefficients presented in Table 6. Also, in order to maintain the relative error at a maximum value of 15%, two ranges of temperature were established, one between 273.15 - 303.15 K and one between 303.15 - 373.15 K.

$$QF_{Coefficient} = x + y \cdot T + z \cdot T^2 \quad \textbf{(7')}$$

$$\eta = QM_a + QM_b \cdot \ln\left(T\right)^{\frac{1}{QM_c}} \quad \textbf{(8')}$$

For the first temperature range, the relative error of equation generated for glycerol dynamic viscosity variation at concentrations between 0% and 65% was -0.25% in overall average and 2.35% in absolute value (maximum individual value: 8.8%) with a R^2 of 0.998. For glycerol concentrations between 65% and 90%, $\varepsilon_{\%}$ was 2.29 and 2.91 in absolute value (9.7% max.) at an R^2 of 0.999.

For the second level of temperature, at a correlation coefficient of 0.999, relative error registered values of -0.3 respectively 1.03 in absolute value (5.0% max.). For the last concentration range (90% to 100%), the relative error reached values of -0.41 (8.14 in absolute and 17.16% max.) for temperature between 273.15 - 323.15 K and -0.05 (0.69 in absolute and 2.25% max.) for temperatures between 323.15 - 373.15 K. In these cases, a R^2 of 0.976 and 0.999 were registered.

The ANOVA analysis, for all generated models, indicated no statistical difference between tabular and calculated data.

As a closing remark, the combination of the developed models for glycerol solutions density and dynamic viscosity, is useful if the kinematic viscosity, *v* [$m^2 \cdot s^{-1}$] (equation 9') is necessary.

$$\nu = \frac{\mu}{\rho} \quad \textbf{(9')}$$

4. Conclusion

The present paper was directed to study the possibility of establishing mathematical correlations between two thermophysical properties of glycerol aqueous solutions (density and dynamic viscosity) and state parameters such as temperature and concentration. These correlations can be useful when design and optimization of industrial equipment or storing, organizing and manipulating data both for industrial and academic users are required.

The various realized attempts of employing the existing values (in tabular or graphical form) as inputs into different software leaded to complex equations which took in consideration only the exact points without respecting the general tendency. More simple and easy to use mathematical expressions were obtained when various computer tools were combined. Statistical analysis of the resulted models showed a high degree of accuracy. For glycerol density, the relative error final overall average was 0.003% while for dynamic density evolution with concentration and temperature, this item reached a maximum of 2.29. In both cases correlation coefficient was higher than 0.99 and the ANOVA test revealed no statistical differences between tabular and calculated data.

Compliance with Ethics Requirements. Authors declare that they respect the journal's ethics requirements. Authors declare that they have no conflict of interest and all procedures involving human / or animal subjects (if exist) respect the specific regulation and standards.

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