Comparing Some Models for Predicting the Density of Liquid Mixtures

MARIA MAGDALENA BUDEANU, SIMONA RADU, VASILE DUMITRESCU*
Petroleum and Gas University of Ploiesti, 39 Bucureşti Blv., 100680, Ploiesti, Romania

The Mchaweh–Nasrifar-Mashfeghian, Hankinson - Thomson, Yamada - Gunn and Reid et al. models were used to estimate the liquid density of the binary mixtures methyl tert-butyl ether (MTBE) + (n-hexane, n-heptane, benzene and tert-butyl alcohol (TBA)) at the range 288.15-313.15 K and atmospheric pressure, over the whole concentration range. All the four theoretical models studied in this work predict with accuracy the liquid density of pure compounds. The Mchaweh–Nasrifar-Mashfeghian model gave the best results for all mixtures, and Yamada - Gunn correlation with the mixing rules proposed in this work gave also accurate results only for MTBE+(n-hexane, n-heptane and benzene).

Key words: density, binary liquid mixtures, theoretical models

Density is an important physical property used in calculating of the molar refraction, parachor and the dipole moment. Also, the density of liquids is used to estimate other physical properties such as boiling temperature, viscosity and superficial tension. The correct values of liquid density are important because they are involved in the equations of heat, mass, and momentum transfer. Knowledge of the density at varied temperature and pressure conditions is necessary in calculations of design equipment and to simulate the physico-chemical processes. The density of liquids can be determined experimentally, but may be correlated and estimated by different analytical relations. These analytical expressions and models are usually based on adjustable parameters for each fluid and on the group contribution methods [1]. Many expressions for predicting the liquid density are based on the corresponding state principle [2-9].

Methyl *tert*-butyl ether (MTBE) and 2-Methyl-2-propanol (TBA) are two oxygenated compounds included in reformulated gasoline to raise the octane number. In this work, four models are applied to estimate the liquids density of the binary mixtures methyl *tert*-butyl ether (MTBE) + *n*-hexane, *n*-heptane, benzene and *tert*-butyl alcohol (TBA) respectively, at the range 288.15-313.15 K and atmospheric pressure, over the whole concentration range.

Theoretical models

Mchaweh–Nasrifar-Mashfeghian model

Mchaweh, Nasrifar and Mashfeghian (M-N-M) [9-11] reported the following correlation:

$$\rho_{mix} = \rho_{cmix}\rho_{0mix} \quad (1)$$

where ρ_{mix} is the solution density, and ρ_{mix} is the critical density of the mixture.

The critical density of the mixture is calculated with the following equation:

$$\rho_{cmix} = \left[\sum_{i=1}^{N} x_i \rho_{ci}^{-3/4}\right]^{-4/3} \quad (2)$$

where x_i is the molar fraction, and ρ_{ci} is the critical density of the *i* component.

The parameter ρ_{0mix} is the reference density of the mixture and calculated with the following equation:

$$\rho_{0mix} = 1 + 1.169\tau_{mix}^{1/3} + 1.818\tau_{mix}^{2/3} - 2.658\tau_{mix}^{3/3} + 2.161\tau_{mix}^{4/3} \quad (3)$$

where the temperature-dependent variable τ_{mix} is calculated by the following expression:

$$\tau_{mix} = 1 - \frac{T_{rmix}}{\alpha_{SRK}} \quad (4)$$

In equation (4) T_{rmix} is the reduced temperature of the mixture and α_{SRK} is the term from the original Soave-Redlich-Kwong equation of state. The reduced temperature of the mixture is defined as:

$$T_{rmix} = \frac{T}{\sum_{i=1}^{N} x_i T_{ci}} \quad (5)$$

where T_{ci} is the critical temperature of the *i* component.

The parameter α_{SRK} is defined in term of reduced temperature (T_r):

$$\alpha_{SRK} = \left[1 + m\left(1 - \sqrt{T_{rmix}}\right)\right]^2 \quad (6)$$

where *m* is calculated with equation (7):

$$m = 0.480 + 1.574\omega_{mix} - 0.176\omega_{mix}^2 \quad (7)$$

The acentric factor of the solution ω_{mix} is calculated with the following expression:

$$\omega_{mix} = \sum_{i=1}^{N} x_i \omega_i \quad (8)$$

where ω_i is the acentric factor of the *i* component. The acentric factor is a measure of the complexity of the molecule as form in relation to a molecule with spherical symmetry of a simple fluid for which $\omega = 0$.

Hankinson and Thomson model

Hankinson - Thomson model (H-T) [12] is based on the corresponding state principle and is valid for $0.25 < T_r < 0.95$. The density of the pure compound is defined by:

$$\rho = \frac{\rho_c}{\left[V^{(0)}\left(1 - \omega V^{(1)}\right)\right]} \quad (9)$$

where $V^{(o)}$ and $V^{(1)}$ are calculated with the following equations:

* email: vdumi@upg-ploiesti.ro

$$V^{(0)} = 1 - 1.5281(1-T_r)^{1/3} + 1.4390(1-T_r)^{2/3} - \\ - 0.8144(1-T_r) + 0.19045(1-T_r)^{4/3} \quad (10)$$

$$V^{(1)} = \left(-0.296123 + 0.386914T_r - 0.0427258T_r^2 - \right. \\ \left. - 0.0480645T_r^3\right)/(T_r - 1.00001) \quad (11)$$

The reduced temperature of the component is defined as:

$$T_r = \frac{T}{T_c} \quad (12)$$

Yamada and Gunn model

Yamada - Gunn model (Y-G) [13] extended the Racket equation and requires the molecular weight M, the critical density ρ_c, the reduced temperature T_r and the acentric factor ω:

$$\rho = \rho_c\left(0.29056 - 0.08775\omega\right)^{-(1-T_r)^{2/7}} \quad (13)$$

Reid et al. model

Reid et al. (R-R) [14] model proposed an equation based also on the molecular weight, critical density, reduced temperature and acentric factor:

$$\rho = \rho_c\left[1 + 0.85(1-T_r) + (1.6916 + 0.984\omega)(1-T_r)^{1/3}\right] \quad (14)$$

The mixing rules

In order to extend the Hankinson - Thomson, Yamada - Gunn, and Reid et. al models to multicomponent systems, we propose the following mixing rules, based on Kay rule [15]:

$$\rho_{cmix} = \sum_{i=1}^{N} x_i \rho_i \quad (15)$$

$$T_{rmix} = \frac{T}{\sum_{i=1}^{N} x_i T_{ci}} \quad (16)$$

$$\omega_{mix} = \sum_{i=1}^{N} x_i \omega_i \quad (17)$$

The acentric factors of the components were obtained [16] by the following equation:

$$\omega = \frac{3}{7}\frac{\lg p_c}{\frac{T_c}{T_f}} - 1 \quad (18)$$

where:

p_c is the critical pressure (atm);

T_c - critical temperature (K);

T_f - boiling temperature (K) at p = 1 atm.

Results and discussion

The densities for the pure compounds and liquid mixtures studied in this work and details about the experimental technique were presented in previously published works [17-19]. In order to evaluate the accuracy of the M-N-M, H-T, Y-G, and R-R models, the liquid density of the pure compounds and of the mixtures were calculated at each experimental temperature and compared with the experimental density. The critical properties of the pure components were taken from the literature [20] and are presented in table 1. This table contents also the acentric factors for studied compounds.

Table 1

CRITICAL PROPERTIES FOR THE COMPONENTS OF THE BINARY SOLUTIONS

Compound	$T_c(K)$	$\rho_c(gcm^{-3})$	ω
MTBE	497.10	0.268	0.266
n-Hexane	507.95	0.234	0.297
n-Heptane	539.95	0.234	0.360
Benzene	561.65	0.304	0.219
TBA	508.15	0.270	0.611

Table 2

LDPD FOR PREDICTION OF LIQUID DENSITY OF PURE COMPOUNDS USING DIFFERENT THEORETICAL MODELS

MTBE			*n* – heptane			*n* - hexane		
T, K	Model	LDPD	T, K	Model	LDPD	T, K	Model	LDPD
	MNM	0.44		MNM	0.95		MNM	0.38
288.15	HT	1.92	288.15	HT	1.92	288.15	HT	1.46
	YG	0.55		YG	0.83		YG	0.17
	RR	1.42		RR	1.64		RR	1.08
	MNM	0.47		MNM	1.08		MNM	0.29
293.15	HT	1.94	293.15	HT	3.45	293.15	HT	1.53
	YG	0.55		YG	0.61		YG	0.18
	RR	1.40		RR	1.40		RR	1.06
	MNM	0.48		MNM	1.10		MNM	0.24
298.15	HT	1.94	298.15	HT	1.70	298.15	HT	1.42
	YG	0.50		YG	0.48		YG	0.17
	RR	1.37		RR	1.30		RR	1.05
	MNM	0.47		MNM	1.20		MNM	0.46
303.15	HT	1.89	303.15	HT	1.60	303.15	HT	1.50
	YG	0.48		YG	0.37		YG	0.17
	RR	1.33		RR	1.20		RR	1.04
	MNM	0.44		MNM	1.20		MNM	0.19
308.15	HT	1.89	308.15	HT	1.40	308.15	HT	1.55
	YG	0.43		YG	0.24		YG	0.17
	RR	1.27		RR	1.07		RR	1.04

Table 3
LDPD FOR PREDICTION OF LIQUID DENSITY OF PURE COMPOUNDS USING DIFFERENT THEORETICAL MODELS

Benzene			TBA		
T, K	Model	LDPD	T, K	Model	LDPD
288.15	MNM	0.31	298.15	MNM	0.40
	HT	0.84		HT	6.60
	YG	0.48		YG	5.80
	RR	0.43		RR	6.60
293.15	MNM	0.25	303.15	MNM	0.45
	HT	0.85		HT	6.50
	YG	0.42		YG	5.80
	RR	0.44		RR	6.00
298.15	MNM	0.22	308.15	MNM	0.56
	HT	0.89		HT	6.50
	YG	0.44		YG	5.70
	RR	0.44		RR	6.00
303.15	MNM	0.22	313.15	MNM	0.58
	HT	0.90		HT	6.40
	YG	0.45		YG	5.60
	RR	0.40		RR	5.90
308.15	MNM	0.21			
	HT	0.90			
	YG	0.47			
	RR	0.37			

In order to compare the Mchaweh–Nasrifar-Mashfeghian, Hankinson - Thomson, Yamada - Gunn, and Reid et al. models used to estimate the liquid density for pure compounds, the liquid density percent deviation (LDPD) were calculated with the equation [10]:

$$LDPD = \left(\frac{|\rho_{calc} - \rho_{exp}|}{\rho_{exp}} \right) \cdot 100 \quad (19)$$

Tables 2 and 3 shows the values of the LDPD calculated for pure components for all the models studied in this work.

Studying the results from tables 2 and 3, some observations are possible:

- all the four theoretical models studied in this work predict with accuracy the liquid density of the MTBE, *n*-hexane, *n*-heptane and benzene (LDPD < 1.94);
- the M-N-M model is the best to estimate the density of MTBE, *n*-hexane and *n*-heptane and Y-G correlation is the second;
- for benzene the M-N-M model is the most accurate and the R-R correlation is the second;
- the M-N-M model is also the best to estimate the density of TBA (LDPD < 0.56) while other correlations show poor and comparable accuracy.

Tables 4-7 present the comparisons of the the Mchaweh–Nasrifar-Mashfeghian, Hankinson - Thomson, Yamada - Gunn, and Reid et al. models applied to estimate the liquid density for MTBE+*n*-hexane, MTBE+*n*-heptane, MTBE+benzene and MTBE+TBA respectively.

The values of the liquid density calculated ρ_{calc} with the four models presented in this work have been compared with the experimental values of this property ρ_{exp} by using the root mean square deviation σ [11]:

$$\sigma = \left(\frac{\sum_{i=1}^{n_{DAT}} (\rho_{exp} - \rho_{calc})^2}{n_{DAT}} \right)^{1/2} \quad (20)$$

where n_{DAT} is the number of experimental data.

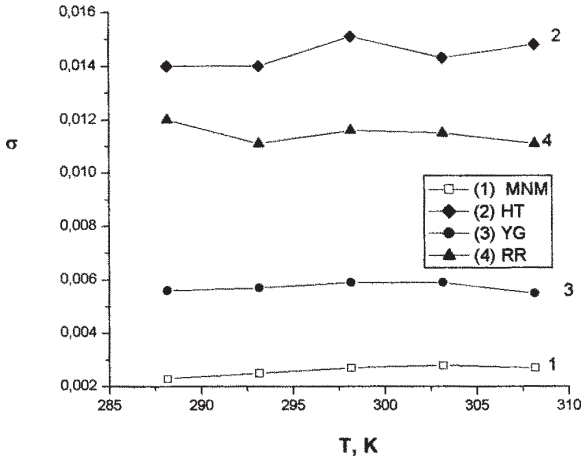

Fig. 1. Root mean square deviation of the density predictions of MTBE + *n*-hexane mixtures

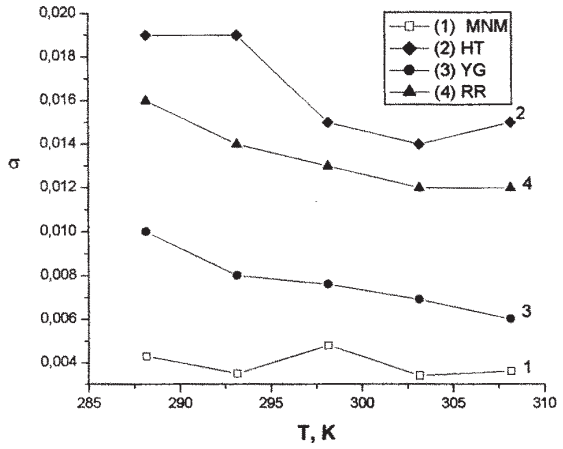

Fig. 2. Root mean square deviation of the density predictions of MTBE + *n*-heptane mixtures

Figure 1-4 are root mean square deviations plot for the M-N-M, H-T, Y-G, and R-R models for the prediction of liquids density of MTBE + *n*-hexane, MTBE + *n*-heptane, MTBE + benzene and MTBE + TBA respectively. The data presented in tables 4-7 and in figures 1-4 reveal that:

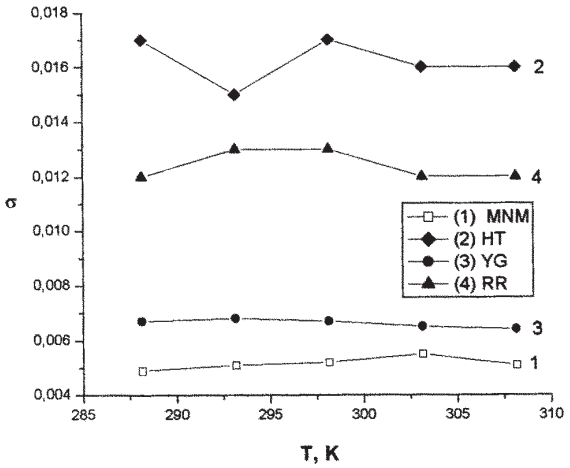

Fig. 3. Root mean square deviation of the density predictions of MTBE + benzene mixtures

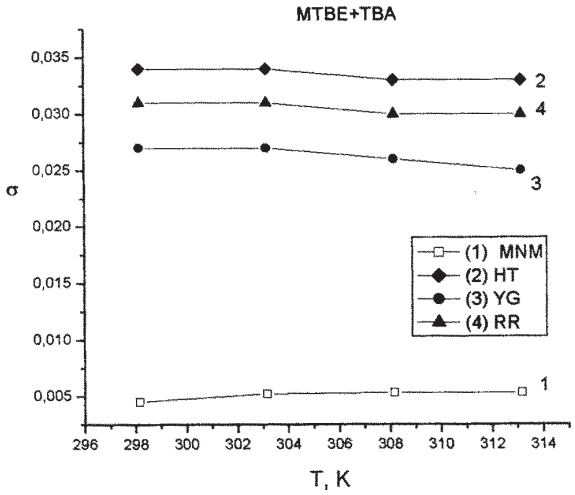

Fig. 4. Root mean square deviation of the density predictions of MTBE + TBA mixtures

Table 4

LIQUID DENSITY OF THE MTBE+ *n*-HEXANE CALCULATED WITH M-N-M, H-T, Y-G, AND R-R EQUATIONS

MTBE + *n*-Hexane									
x	ρ^{MNM}_{calc}	ρ^{HT}_{calc}	ρ^{YG}_{calc}	ρ^{RR}_{calc}	x	ρ^{MNM}_{calc}	ρ^{HT}_{calc}	ρ^{YG}_{calc}	ρ^{RR}_{calc}
		288.15K					293.15K		
0.0000	0.6629	0.6751	0.6665	0.6722	0.0000	0.6587	0.6707	0.6618	0.6676
0.1085	0.6713	0.6842	0.6757	0.6816	0.1085	0.6670	0.6795	0.6711	0.6769
0.2044	0.6790	0.6929	0.6841	0.6899	0.2044	0.6746	0.6882	0.6793	0.6851
0.2976	0.6867	0.7013	0.6922	0.6980	0.2976	0.6822	0.6963	0.6873	0.6785
0.4079	0.6944	0.7103	0.7013	0.7073	0.4079	0.6899	0.7061	0.6963	0.7024
0.4981	0.7038	0.7179	0.7086	0.7148	0.4981	0.6991	0.7130	0.7036	0.7098
0.5969	0.7124	0.7264	0.7169	0.7233	0.5969	0.7078	0.7214	0.7119	0.7181
0.6978	0.7213	0.7352	0.7253	0.7317	0.6978	0.7165	0.7300	0.7202	0.7265
0.8091	0.7314	0.7387	0.7348	0.7410	0.8091	0.7265	0.7393	0.7296	0.7358
0.9027	0.7404	0.7526	0.7425	0.7490	0.9027	0.7354	0.7471	0.7373	0.7436
1.0000	0.7497	0.7607	0.7505	0.7570	1.0000	0.7447	0.7556	0.7453	0.7516
		298.15K					303.15K		
0.0000	0.6544	0.6653	0.6571	0.6629	0.0000	0.6484	0.6612	0.6525	0.6582
0.1085	0.6627	0.6751	0.6664	0.6721	0.1085	0.6583	0.6705	0.6617	0.6673
0.2044	0.6702	0.6833	0.6745	0.6803	0.2044	0.6657	0.6785	0.6696	0.6755
0.2976	0.6776	0.6916	0.6825	0.6883	0.2976	0.6731	0.6865	0.6776	0.6833
0.4079	0.6853	0.7005	0.6915	0.6973	0.4079	0.6806	0.6956	0.6865	0.6923
0.4981	0.6944	0.7078	0.6987	0.7047	0.4981	0.6897	0.7034	0.6937	0.6996
0.5969	0.7030	0.7165	0.7070	0.7131	0.5969	0.6981	0.7113	0.7017	0.7078
0.6978	0.7117	0.7249	0.7152	0.7213	0.6978	0.7067	0.7169	0.7101	0.7160
0.8091	0.7216	0.7358	0.7257	0.7305	0.8091	0.7166	0.7226	0.7213	0.7261
0.9027	0.7304	0.7421	0.7320	0.7383	0.9027	0.7252	0.7365	0.7268	0.7328
1.0000	0.7395	0.7503	0.7397	0.7461	1.0000	0.7343	0.7447	0.7344	0.7406
		308.15K							
0.0000	0.6455	0.6567	0.6478	0.6534					
0.1085	0.6537	0.6656	0.6568	0.6625					
0.2044	0.6611	0.6737	0.6648	0.6705					
0.2976	0.6684	0.6817	0.6727	0.6783					
0.4079	0.6758	0.6909	0.6816	0.6873					
0.4981	0.6848	0.6981	0.6885	0.6944					
0.5969	0.6913	0.7064	0.6971	0.7026					
0.6978	0.7017	0.7144	0.7049	0.7107					
0.8091	0.7115	0.7240	0.7139	0.7197					
0.9027	0.7200	0.7316	0.7213	0.7272					
1.0000	0.7290	0.7395	0.7289	0.7350					

- the M-N-M theoretical model is the best to predict the liquid density of the mixtures studied in this work;
- the accuracy of the studied models follows the sequence: M-N-M>Y-G>R-R>H-T;
- MTBE+TBA mixture values of root mean square deviations calculated with H-T, Y-G and R-R models are an order size higher than those calculated with M-N-M correlation;
- for the MTBE+(*n*-hexane, *n*-heptane and benzene) systems the values of root mean square deviations calculated with M-N-M and Y-G models have the same order of size and are smaller than the values calculated with the other correlations;

Table 5
LIQUID DENSITY OF THE MTBE+ *n*-HEPTANE CALCULATED WITH M-N-M, H-T, Y-G, AND R-R EQUATIONS

MTBE + *n*-Heptane									
x	ρ_{calc}^{MNM}	ρ_{calc}^{HT}	ρ_{calc}^{YG}	ρ_{calc}^{RR}	x	ρ_{calc}^{MNM}	ρ_{calc}^{HT}	ρ_{calc}^{YG}	ρ_{calc}^{RR}
		288.15K					293.15K		
0.0000	0.6811	0.7008	0.6933	0.6989	0.0000	0.6774	0.6612	0.6890	0.6813
0.1978	0.6949	0.7136	0.7057	0.7114	0.1978	0.6907	0.7094	0.7011	0.7069
0.3948	0.7070	0.7257	0.7173	0.7235	0.3948	0.7037	0.7213	0.7126	0.7188
0.4882	0.7140	0.7319	0.7230	0.7291	0.4882	0.7073	0.7270	0.7183	0.7243
0.6022	0.7221	0.7385	0.7294	0.7357	0.6022	0.7175	0.7339	0.7245	0.7307
0.7996	0.7356	0.7497	0.7402	0.7466	0.7996	0.7308	0.7448	0.7349	0.7414
1.0000	0.7497	0.7607	0.7505	0.7570	1.0000	0.7447	0.7556	0.7453	0.7516
		298.15 K					303.15K		
0.0000	0.6736	0.6929	0.6846	0.6903	0.0000	0.6698	0.6886	0.6802	0.6860
0.1978	0.6869	0.7044	0.6967	0.7024	0.1978	0.6828	0.7003	0.6921	0.6978
0.3948	0.7071	0.7169	0.7079	0.7141	0.3948	0.6951	0.7121	0.7030	0.7093
0.4882	0.7053	0.7222	0.7134	0.7194	0.4882	0.7008	0.7174	0.7085	0.7145
0.6022	0.7130	0.7288	0.7195	0.7258	0.6022	0.7084	0.7238	0.7145	0.7207
0.7996	0.7260	0.7241	0.7290	0.7362	0.7996	0.7210	0.7347	0.7248	0.7309
1.0000	0.7395	0.7503	0.7397	0.7461	1.0000	0.7343	0.7447	0.7344	0.7406
		308.15K							
0.0000	0.6659	0.6838	0.6759	0.6815					
0.1978	0.6786	0.6959	0.6873	0.6932					
0.3948	0.6907	0.7081	0.6983	0.7044					
0.4882	0.6963	0.7127	0.7035	0.7095					
0.6022	0.7036	0.7187	0.7075	0.7157					
0.7996	0.7161	0.7292	0.7194	0.7256					
1.0000	0.7290	0.7395	0.7289	0.7350					

Table 6
LIQUID DENSITY OF THE MTBE+ BENZENE CALCULATED WITH M-N-M, H-T, Y-G, AND R-R EQUATIONS

MTBE + Benzene									
x	ρ_{calc}^{MNM}	ρ_{calc}^{HT}	ρ_{calc}^{YG}	ρ_{calc}^{RR}	x	ρ_{calc}^{MNM}	ρ_{calc}^{HT}	ρ_{calc}^{YG}	ρ_{calc}^{RR}
		288.15K					293.15K		
0.0000	0.8806	0.8907	0.8791	0.8871	0.0000	0.8758	0.8855	0.8743	0.8819
0.1055	0.8629	0.8747	0.8629	0.8706	0.1055	0.8580	0.8694	0.8577	0.8654
0.2081	0.8515	0.8642	0.8527	0.8604	0.2081	0.8469	0.8594	0.8479	0.8561
0.3016	0.8391	0.8518	0.8408	0.8482	0.3016	0.8343	0.8469	0.8356	0.8431
0.4056	0.8253	0.8388	0.8278	0.8196	0.4056	0.8206	0.8335	0.8226	0.8300
0.5010	0.8128	0.8290	0.8155	0.8228	0.5010	0.8080	0.8211	0.8104	0.8175
0.6095	0.7986	0.8120	0.8011	0.8083	0.6095	0.7936	0.8066	0.7959	0.8029
0.7025	0.7868	0.8002	0.7893	0.7963	0.7025	0.7820	0.7785	0.7842	0.7910
0.8049	0.7738	0.7862	0.7760	0.7827	0.8049	0.7689	0.7810	0.7712	0.7772
0.9058	0.7615	0.7732	0.7628	0.7695	0.9058	0.7564	0.7678	0.7575	0.7650
1.0000	0.7497	0.7607	0.7505	0.7570	1.0000	0.7447	0.7556	0.7453	0.7516
		298.15K					303.15K		
0.0000	0.8712	0.8809	0.8693	0.8769	0.0000	0.8664	0.8761	0.8644	0.8718
0.1055	0.8534	0.8646	0.8528	0.8601	0.1055	0.8485	0.8594	0.8475	0.8549
0.2081	0.8420	0.8542	0.8426	0.8501	0.2081	0.8373	0.8488	0.8376	0.8443
0.3016	0.8295	0.8418	0.8308	0.8379	0.3016	0.8247	0.8370	0.8256	0.8327
0.4056	0.8157	0.8286	0.8177	0.8248	0.4056	0.8108	0.8236	0.8125	0.8195
0.5010	0.8030	0.8162	0.8052	0.8122	0.5010	0.7981	0.8111	0.8000	0.8069
0.6095	0.7888	0.8018	0.7908	0.7977	0.6095	0.7838	0.7962	0.7857	0.7923
0.7025	0.7768	0.7897	0.7789	0.7856	0.7025	0.7719	0.7844	0.7735	0.7802
0.8049	0.7638	0.7764	0.7654	0.7720	0.8049	0.7587	0.7707	0.7601	0.7665
0.9058	0.7514	0.7628	0.7522	0.7587	0.9058	0.7461	0.7573	0.7468	0.7532
1.0000	0.7395	0.7503	0.7397	0.7461	1.0000	0.7343	0.7447	0.7344	0.7406
		308.15K							
0.0000	0.8615	0.8711	0.8592	0.8665					
0.1055	0.8435	0.8536	0.8425	0.8496					
0.2081	0.8324	0.8438	0.8324	0.8396					
0.3016	0.8197	0.8317	0.8205	0.8273					
0.4056	0.8059	0.8184	0.8073	0.8142					
0.5010	0.7930	0.8063	0.7949	0.8015					
0.6095	0.7787	0.7910	0.7803	0.7869					
0.7025	0.7668	0.7791	0.7684	0.7748					
0.8049	0.7535	0.7654	0.7547	0.7610					
0.9058	0.7409	0.7522	0.7415	0.7477					
1.0000	0.7290	0.7395	0.7289	0.7350					

- there is no systematic influence of temperature on root mean square deviations.

Table 7
LIQUID DENSITY OF THE MTBE+ TBA CALCULATED WITH M-N-M, H-T, Y-G, AND R-R EQUATIONS

MTBE + TBA									
x	ρ^{MNM}_{calc}	ρ^{HT}_{calc}	ρ^{YG}_{calc}	ρ^{RR}_{calc}	x	ρ^{MNM}_{calc}	ρ^{HT}_{calc}	ρ^{YG}_{calc}	ρ^{RR}_{calc}
		298.15K					303.15K		
0.0000	0.7835	0.8318	0.8259	0.8274	0.0000	0.7786	0.8257	0.8197	0.8214
0.0968	0.7793	0.8228	0.8168	0.8193	0.0968	0.7744	0.8171	0.8107	0.8135
0.1976	0.7756	0.8143	0.8072	0.8111	0.1976	0.7707	0.8080	0.8012	0.8052
0.3014	0.7715	0.8054	0.7980	0.8026	0.3014	0.7665	0.7999	0.7921	0.7969
0.4022	0.7672	0.7976	0.7890	0.7945	0.4022	0.7622	0.7913	0.7830	0.7887
0.4990	0.7630	0.7891	0.7806	0.7865	0.4990	0.7580	0.7833	0.7748	0.7809
0.6031	0.7584	0.7807	0.7720	0.7781	0.6031	0.7533	0.7746	0.7662	0.7725
0.6988	0.7522	0.7732	0.7639	0.7708	0.6988	0.7489	0.7674	0.7583	0.7647
0.8021	0.7473	0.7649	0.7554	0.7621	0.8021	0.7440	0.7593	0.7499	0.7564
0.9111	0.7422	0.7566	0.7467	0.7533	0.9111	0.7388	0.7515	0.7413	0.7478
1.0000	0.7395	0.7503	0.7397	0.7461	1.0000	0.7343	0.7447	0.7344	0.7406
		308.15K					313.15K		
0.0000	0.7737	0.8192	0.8133	0.8154	0.0000	0.7686	0.8130	0.8069	0.8094
0.0968	0.7695	0.8109	0.8044	0.8075	0.0968	0.7643	0.8044	0.7980	0.8015
0.1976	0.7656	0.8024	0.7950	0.7994	0.1976	0.7606	0.7960	0.7888	0.7934
0.3014	0.7614	0.7933	0.7859	0.7910	0.3014	0.7562	0.7875	0.7797	0.7851
0.4022	0.7570	0.7855	0.7791	0.7828	0.4022	0.7519	0.7794	0.7711	0.7770
0.4990	0.7528	0.7772	0.7690	0.7750	0.4990	0.7475	0.7717	0.7629	0.7692
0.6031	0.7480	0.7693	0.7604	0.7667	0.6031	0.7429	0.7636	0.7544	0.7609
0.6988	0.7437	0.7616	0.7526	0.7590	0.6988	0.7383	0.7562	0.7467	0.7532
0.8021	0.7387	0.7541	0.7443	0.7508	0.8021	0.7334	0.7480	0.7384	0.7451
0.9111	0.7335	0.7488	0.7358	0.7422	0.9111	0.7282	0.7403	0.7302	0.7365
1.0000	0.7290	0.7395	0.7289	0.7350	1.0000	0.7236	0.7395	0.7233	0.7294

Conclusions

Four theoretical models were studied to predict the liquid density of MTBE+(*n*-hexane, *n*-heptane, benzene and TBA) at the range 288.15-313.15 K and atmospheric pressure, over the whole concentration range. All theoretical models studied in this work predict with accuracy the liquid density of the pure compounds. The M-N-M correlation shows the best results for all mixtures investigated. The Y-G model with the mixing rules proposed in this work gives also accurate results for MTBE+(*n*-hexane, *n*-heptane and benzene). The accuracy of the studied models for the binary mixtures analyzed in this work follows the sequence: M-N-M>Y-G>R-R>H-T.

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