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A simple accurate model for prediction of physical properties of petroleum fractions

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Abstract−We utilized genetic programming approach for generation of a new model for prediction of critical properties and acentric factor of petroleum fractions. Usually for estimation of critical properties, molecular weight, specific gravity and boiling point are needed, while in this work in order to present an applicable model, just the boiling point and specific gravity have been used as the model parameters. Our results showed that using new correlations, critical temperature, pressure, volume and acentric of petroleum fractions can be correlated within 0.07, 0.65, 0.45 and 0.79 percent average absolute relative deviation. respectively.

Keywords: Genetic Programming, Critical Properties, Acentric Factor, Petroleum Fraction

INTRODUCTION

Critical properties and acentric factors of petroleum fractions are accounted as the most essential properties for thermodynamic calculations in reservoir engineering [1-5]. They are widely used in corresponding states theories, calculation of thermo-physical properties such as heat capacity, enthalpy of vaporization, compressibility factor, vapor pressure, interfacial tension and viscosity [6-14]. Recently, He and Ghoniem [15] and Xu et al. [16] utilized the critical properties and acentric factor to develop a new model for predicting binary-interaction parameters (K_{ij}) of petroleum fluids. Petroleum fractions usually contain aromatics, aliphatic hydrocarbons as well as non-hydrocarbon materials such as N2, and H2S with unknown composition [6,11,13,17]. For this reason, estimation of critical properties of petroleum fractions is considered as a complex problem. In the past few years, numerous methods have been presented for estimation of critical properties and acentric factors of petroleum fractions. Among various methods, those approaches which need petroleum composition as a basic data cannot be utilized in many cases. Lee and Kessler proposed some correlations based on bulk properties (normal boiling point and specific gravity) for calculation of critical temperature and critical pressure. In their method, the acentric factor is estimated using critical temperature, critical pressure and normal boiling point [6,8,13]. Cavett proposed a correlation in which normal boiling point and API are used as input parameters for estimation of critical temperature and critical pressure [18]. Edmister generated a new model for estimation of acentric factor as a function of critical pressure, critical temperature and normal boiling point temperature [19]. Riazi and Daubert generated a general function for estimation of different properties. They used normal boiling point, molecular weight and specific gravity as input parameters [11-13]. Twu presented a method which initially correlates the properties of normal paraffins as the reference [20], then the estimated values are utilized for petroleum fractions which have the same boiling point temperature. Mohammadi et al. proposed a new model based on the artificial neural network (ANN) technique to predict the critical properties and acentric factors of petroleum fractions, especially heavy fractions. In their method specific gravity and average normal boiling-point temperature are used as input data [10].

In most of the previous methods, physical properties of pure and light hydrocarbons have been used as databank; therefore, they may fail in estimation of properties of heavy petroleum fractions. Hence, there is strong demand for accurate methods which can calculate heavy hydrocarbons properties. In recent years quantitative structure property relationship (QSPR) and group contribution (GC) approaches have been proposed to calculate critical properties and acentric factors of pure compounds [7,14], although these approaches are not applicable for petroleum fractions, as there are hundreds of compounds in petroleum fractions and huge calculation is required.

Alternatively, genetic programming (GP) has been already used in chemical engineering such as determination of kinetic orders, optimization of complex distillation systems [21-24]. Shokir utilized a genetic programming approach combined with orthogonal least squares algorithm (GP-OLS) to estimate the compressibility factor of sweet, sour, and condensate gases [25]. In another work GP-OLS was used by Shokir for estimation of viscosity of pure and hydrocarbon gas mixtures [26]. In a similar work AlQuraish utilized a linear genetic programming to determinate the saturation pressure of crude oil [27]. Recent works indicate that the GP approach is successful in estimation of compressibility factor, viscosity and saturation pressure. In our previous work, GP was utilized to develop the new model for prediction of vaporization enthalpy of petroleum fractions as well as pure hydrocarbons [28].

This work aims at showing how genetic programming method

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is capable of generating a new accurate model for predicting critical properties and acentric factors of petroleum fractions. GP is known to be a robust and predictive method in modeling nonlinear complex systems. To our knowledge, GP methods have not previously been reported for accurately estimating the critical properties and acentric factors of petroleum fractions. Our new model has been constructed as function of normal boiling point temperatures (T_b) and specific gravity (S). To generate these models, the available experimental data in the literature [6,10] on the critical properties and acentric factors of petroleum fractions have been used. In the first section of this work, the methodology and modeling with GP is presented, then the results are compared with previous works.

GENETIC PROGRAMMING

1. Theory

Genetic programming is a member of the evolutionary algorithms advanced by Koza; it is categorized as a subclass of genetic algorithms (GA). GP has been developed in evolutionary algorithms by symbolic optimization [29]. GP and GA are different in search space and population structures [30-32]. Search space and population structure in the GP is a computer program and tree structure, respectively, while in the GA, search space and population structures are constant. The flexibility of tree structure helps GP to reproduce nonlinear input-output empirical models for prediction of thermo-physical properties. This structure entails two main sets, function and terminal sets. The function set can contain the arithmetic operator [33] or even may also be made up of Boolean functions, conditional statements ("if…", "then…"), trigonometric functions, iterative functions, recursive functions and other mathematical functions [34]. The terminal set comprises independent variables, numerical constants and other zero-argument in the GP tree [29,31]. Calculation starts when the initial population of GP is determined. GA and GP methods are very similar in programming structure and genetic operators. In the first step, the fitness of each individual is evaluated. Then a new population is randomly generated using the current population and based on Darwin's principles, such as crossover, reproduction and mutation. For the next generation, genetic operators such as selection, replacement, mutation and crossover are used for producing a new population. Many selection methods have been proposed as the reproduction operator; however, rank-based selection, tournament selection and roulette-wheel selection are the most common types [34]. It should be mentioned that the reproduction operator helps the best individuals in the current generation survive into next generation [29]. Crossover operator exchanges a part of the structure between two individuals, and the mutation operator changes one individual of the population. These operators increase the population diversity and help to avoid early convergence. To produce new individuals, the individuals with maximum error in the current generation are killed by the replacement operator [34], while the individuals with lower error are reproduced in the next generation. This process will continue to achieve specific error or number of generations [29]. Interested readers can find more details about GP in the following references [29-32,34].

2. Modeling of Critical Properties and Acentric Factors

In this work, the GP technique has been applied to generate new equations for prediction of critical properties and acentric factors of pure hydrocarbons and petroleum fractions. A complete review about available models and correlations was given in the introduction section. Usually, critical properties of petroleum fractions are estimated as a function of specific gravity (S) at 288.7 K, normal boiling point temperatures (T_b) and molecular weight (M). Among the mentioned properties, measurement of molecular weight is difficult and it has considerable uncertainty. Considering this fact, in this work specific gravity and normal boiling point have been utilized as input parameters as they can be measured easily. To start the modeling, two sets of experimental data are required; one set is used for training and the second one is used for testing and evaluating the model. In this regard having a reliable experimental data set is mandatory. Required comprehensive experimental data of petroleum fractions (pseudo experimental data) and pure hydrocarbons were obtained from the literature [6,10]. Sixty seven (67) experimental data points have been collected (49 data point for petroleum fractions and remaining data point for pure hydrocarbon). To evaluate the predictive ability of the model, the experimen-

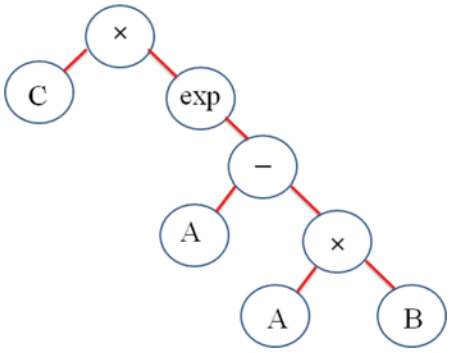

Fig. 1. Tree structure representation of the equation C×exp (A−(A×B)).

Table 1. Maximum and minimum of input parameters utilized for training and testing the critical properties and acentric factor models

Parameter	Training data		Testing data	
	Maximum	Minimum	Maximum	Minimum
Tb(K)	826	112	664.40	371.58
S	0.940	0.300	0.803	0.688

Table 2. GP parameters used in building the new models

Population size	25000
Maximum generation	2000
Type of selection	Roulette wheel
Type of crossover	One point (two parents)
Type of mutation point	One point
Probability of crossover	0.87
Probability of mutation	0.05
probability of reproduction	0.08

Table 3. Comparison of critical temperature calculated by the new model with previous models for petroleum fractions

	Petroleum fraction	Input		Tc/K	Riazi and Daubert [12]		Riazi and Daubert [11]		Lee-Kesler Method [8]		Cavett Method [18]		Twu Method [20]		Winn Method [38]		Tsonopoulos et al. [37]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	C1	112	0.3	190.6	198.64	4.22	178.44	6.38	235.41	23.51	779.23	308.83	200.67	5.28	216.85	13.77	252.09	32.26	190.6	0.00	190.60	0.00
2	C2	185	0.356	305.3	283.83	7.03	271.82	10.96	320.59	5.01	496.23	62.54	298.39	2.26	296.56	2.86	334.06	9.42	305.4	0.03	305.21	0.03
3	C3	231	0.507	369.8	367.31	0.67	358.91	2.95	371.43	0.44	417.46	12.89	370.00	0.05	371.98	0.59	380.86	2.99	369.5	0.08	368.75	0.28
4	i-C4	261	0.563	408.1	409.83	0.42	403.08	1.23	409.52	0.35	430.33	5.45	408.96	0.21	411.38	0.80	415.80	1.89	408	0.02	408.65	0.13
5	n-C4	273	0.584	425.1	426.39	0.30	420.18	1.16	424.92	0.04	439.44	3.37	424.73	0.09	426.82	0.41	430.01	1.16	422.9	0.52	424.46	0.15
6	i-C5	301	0.625	460.4	462.77	0.51	457.79	0.57	460.06	0.07	465.31	1.07	460.18	0.05	461.05	0.14	462.69	0.50	459.9	0.11	460.10	0.06
7	Ne-C5	283	0.597	433.8	438.98	1.19	433.30	0.11	437.26	0.80	447.84	3.24	436.80	0.69	438.68	1.12	441.40	1.75	435.8	0.46	436.91	0.72
8	N-C5	309	0.631	469.7	471.58	0.40	467.09	0.56	469.18	0.11	472.81	0.66	468.84	0.18	469.50	0.04	471.21	0.32	469.7	0.00	469.13	0.12
9	n-C6	342	0.664	507.6	509.86	0.45	506.84	0.15	507.45	0.03	507.05	0.11	507.31	0.06	506.16	0.28	507.66	0.01	509.3	0.33	507.60	0.00
10	C6	337	0.69	509.9	512.49	0.51	508.22	0.33	507.63	0.44	507.49	0.47	510.16	0.05	507.90	0.39	507.98	0.38	509.7	0.04	509.82	0.02
11	C7	366	0.727	547.2	548.20	0.18	544.80	0.44	543.32	0.71	542.04	0.94	546.57	0.12	542.14	0.92	542.54	0.85	546.4	0.15	546.92	0.05
12	C8	390	0.749	574.1	575.21	0.19	572.73	0.24	570.68	0.60	569.60	0.78	574.35	0.04	568.39	0.99	569.46	0.81	574.3	0.03	574.92	0.14
13	C9	416	0.768	603.2	602.89	0.05	601.45	0.29	598.67	0.75	598.48	0.78	602.90	0.05	595.57	1.27	597.47	0.95	602.7	0.08	603.36	0.03
14	C10	439	0.782	626.9	626.34	0.09	625.79	0.18	622.25	0.74	623.16	0.60	627.06	0.03	618.80	1.29	621.46	0.87	626.6	0.05	627.26	0.06
15	C11	461	0.793	649.1	647.87	0.19	648.13	0.15	643.75	0.82	645.87	0.50	649.16	0.01	640.30	1.36	643.65	0.84	648.6	0.08	649.00	0.02
16	C12	482	0.804	670	668.38	0.24	669.31	0.10	664.08	0.88	667.38	0.39	670.12	0.02	660.86	1.36	664.87	0.77	669.4	0.09	669.78	0.03
17	C13	501	0.815	688.9	687.11	0.26	688.59	0.04	682.57	0.92	686.87	0.30	689.22	0.05	679.69	1.34	684.32	0.67	688.4	0.07	688.90	0.00
18	C14	520	0.826	708.2	705.72	0.35	707.73	0.07	700.88	1.03	706.10	0.30	708.15	0.01	698.46	1.38	703.73	0.63	707.2	0.14	707.93	0.04
19	C15	539	0.836	727.1	723.91	0.44	726.41	0.09	718.72	1.15	724.78	0.32	726.57	0.07	716.91	1.40	722.80	0.59	725.6	0.21	726.45	0.09
20	C16	557	0.843	743	740.26	0.37	743.16	0.02	734.65	1.12	741.53	0.20	742.98	0.00	733.64	1.26	740.01	0.40	742.4	0.08	742.80	0.03
21	C17	573	0.851	758.1	755.26	0.37	758.52	0.06	749.30	1.16	756.73	0.18	758.10	0.00	748.98	1.20	755.85	0.30	757.6	0.07	758.05	0.01
22	C18	586	0.856	770	766.91	0.40	770.42	0.05	760.61	1.22	768.52	0.19	769.74	0.03	760.98	1.17	768.18	0.24	769.5	0.06	769.71	0.04
23	C19	598	0.861	781	777.74	0.42	781.47	0.06	771.13	1.26	779.42	0.20	780.57	0.05	772.14	1.13	779.68	0.17	780.6	0.05	780.61	0.05
24	C20	612	0.866	793.2	790.05	0.40	793.98	0.10	783.04	1.28	791.78	0.18	792.82	0.05	784.90	1.05	792.75	0.06	793.2	0.00	792.89	0.04
25	C21	624	0.871	803.7	800.79	0.36	804.92	0.15	793.45	1.28	802.49	0.15	803.55	0.02	796.02	0.96	804.20	0.06	804.1	0.05	803.71	0.00
26	C22	637	0.876	814.7	812.23	0.30	816.55	0.23	804.53	1.25	813.89	0.10	814.95	0.03	807.92	0.83	816.42	0.21	815.7	0.12	815.19	0.06
27	C23	648	0.881	824.9	822.14	0.33	826.66	0.21	814.15	1.30	823.68	0.15	824.88	0.00	818.22	0.81	827.04	0.26	825.7	0.10	825.23	0.04
28	C24	659	0.885	834.3	831.68	0.31	836.33	0.24	823.38	1.31	833.13	0.14	834.37	0.01	828.19	0.73	837.26	0.36	835.5	0.14	834.77	0.06
29	C25	671	0.888	844.1	841.58	0.30	846.27	0.26	832.88	1.33	843.03	0.13	844.13	0.00	838.62	0.65	847.86	0.45	845.4	0.15	844.50	0.05
30	C26	681	0.892	853.3	850.31	0.35	855.14	0.22	841.34	1.40	851.64	0.19	852.86	0.05	847.77	0.65	857.26	0.46	854.1	0.09	853.29	0.00
31	C27	691	0.896	861.7	859.02	0.31	863.98	0.26	849.78	1.38	860.22	0.17	861.58	0.01	856.92	0.56	866.65	0.57	862.7	0.12	862.06	0.04
32	C28	701	0.899	869.9	867.35	0.29	872.36	0.28	857.81	1.39	868.51	0.16	869.85	0.01	865.72	0.48	875.63	0.66	871	0.13	870.33	0.05
33	C29	709	0.902	877	874.21	0.32	879.32	0.26	864.45	1.43	875.28	0.20	876.72	0.03	872.96	0.46	883.04	0.69	877.8	0.09	877.21	0.02
34	C30	719	0.905	885.1	882.50	0.29	887.64	0.29	872.43	1.43	883.54	0.18	884.96	0.02	881.74	0.38	891.99	0.78	886	0.10	885.44	0.04
35	C31	728	0.909	893.3	890.39	0.33	895.71	0.27	880.12	1.48	891.29	0.23	892.96	0.04	890.07	0.36	900.58	0.82	893.7	0.04	893.45	0.02
36	C32	737	0.912	901.4	897.92	0.39	903.30	0.21	887.39	1.55	898.77	0.29	900.50	0.10	898.07	0.37	908.74	0.81	901	0.04	900.95	0.05
37	C33	745	0.915	906.7	904.71	0.22	910.20	0.39	893.98	1.40	905.50	0.13	907.36	0.07	905.27	0.16	916.13	1.04	907.7	0.11	907.77	0.12

Table 3. Continued

	Petroleum fraction	Input		Tc/K	Riazi and Daubert [12]		Riazi and Daubert [11]		Lee-Kesler Method [8]		Cavett Method [18]		Twu Method [20]		Winn Method [38]		Tsonopoulos et al. [37]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
38	C34	753	0.917	914.1	911.13	0.32	916.59	0.27	900.16	1.53	912.00	0.23	913.75	0.04	912.14	0.21	923.09	0.98	914	0.01	914.09	0.00
39	C35	760	0.92	920.4	917.18	0.35	922.79	0.26	906.05	1.56	917.97	0.26	919.92	0.05	918.57	0.20	929.71	1.01	919.9	0.05	920.22	0.02
40	C36	768	0.922	926.2	923.57	0.28	929.15	0.32	912.21	1.51	924.47	0.19	926.30	0.01	925.42	0.08	936.64	1.13	926.2	0.00	926.51	0.03
41	C37	774	0.925	931.9	928.90	0.32	934.66	0.30	917.43	1.55	929.70	0.24	931.80	0.01	931.07	0.09	942.50	1.14	931.9	0.00	931.96	0.01
42	C38	782	0.927	937.6	935.26	0.25	941.00	0.36	923.56	1.50	936.22	0.15	938.18	0.06	937.91	0.03	949.42	1.26	937.6	0.00	938.23	0.07
43	C39	788	0.929	943.2	940.20	0.32	946.00	0.30	928.36	1.57	941.22	0.21	943.20	0.00	943.21	0.00	954.83	1.23	942.4	0.08	943.17	0.00
44	C40	796	0.931	949.6	946.54	0.32	952.31	0.28	934.47	1.59	947.77	0.19	949.58	0.00	950.04	0.05	961.74	1.28	948.7	0.09	949.41	0.02
45	C41	801	0.933	954	950.77	0.34	956.63	0.28	938.60	1.61	952.03	0.21	953.93	0.01	954.56	0.06	966.39	1.30	952.9	0.12	953.67	0.03
46	C42	807	0.934	956.3	955.32	0.10	961.08	0.50	942.96	1.39	956.86	0.06	958.48	0.23	959.50	0.33	971.33	1.57	957.5	0.13	958.09	0.19
47	C43	813	0.936	964.2	960.23	0.41	966.05	0.19	947.74	1.71	961.91	0.24	963.51	0.07	964.79	0.06	976.72	1.30	962.4	0.19	963.00	0.12
48	C44	821	0.938	969.6	966.52	0.32	972.30	0.28	953.82	1.63	968.52	0.11	969.89	0.03	971.60	0.21	983.60	1.44	968.7	0.09	969.19	0.04
49	C45	826	0.94	973.9	970.73	0.33	976.62	0.28	957.93	1.64	972.82	0.11	974.25	0.04	976.12	0.23	988.24	1.47	972.9	0.10	973.44	0.05
				AARD%		**0.56**		**0.68**		**1.66**		**8.34**		**0.21**		**0.95**		**1.65**		**0.10**		**0.07**

[a]Quoted in Mohammadi et al. [10]

Table 4. Comparison of critical pressure calculated by the new model with previous models for petroleum fractions

	Petroleum fraction	Input		Pc/MPa	Riazi and Daubert [12]		Riazi and Daubert [11]		Lee-Kesler Method [8]		Cavett Method [18]		Twu Method [20]		Winn Method [38]		Tsonopoulos et al. [37]		Mohammadi et al. [10]		New model	
		T_b/K	S	Exp.	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%
1	C1	112	0.3	4.599	6.18	34.32	2.64	42.70	4.08	11.34	-	-	10.73	133.32	5.49	19.43	54.99	1095.76	4.60	0.02	4.596	0.070
2	C2	185	0.356	4.872	2.88	40.91	2.06	57.80	2.26	53.70	-	-	4.46	8.43	2.63	46.09	12.94	165.61	4.87	0.10	4.886	0.281
3	C3	231	0.507	4.248	3.91	7.89	3.44	19.00	3.44	19.03	6.46	52.19	4.26	0.31	3.78	11.02	5.96	40.18	4.25	0.05	4.128	2.820
4	i-C4	261	0.563	3.648	3.76	3.13	3.50	4.13	3.43	5.85	4.41	20.98	3.88	6.33	3.70	1.30	4.71	29.20	3.70	1.43	3.798	4.104
5	n-C4	273	0.584	3.796	3.69	2.76	3.49	8.17	3.42	10.01	4.03	6.13	3.75	1.12	3.65	3.93	4.38	15.31	3.58	5.77	3.680	3.051
6	i-C5	301	0.625	3.381	3.45	1.96	3.35	0.96	3.28	2.86	3.49	3.09	3.46	2.32	3.44	1.82	3.77	11.36	3.35	1.06	3.412	0.905
7	Ne-C5	283	0.597	3.199	3.57	11.74	3.42	6.78	3.34	4.55	3.78	18.15	3.63	13.41	3.54	10.78	4.12	28.78	3.48	8.75	3.571	11.635
8	N-C5	309	0.631	3.37	3.32	1.57	3.25	3.68	3.18	5.51	3.35	0.57	3.35	0.52	3.32	1.56	3.59	6.66	3.27	3.09	3.315	1.626
9	n-C6	342	0.664	3.025	2.95	2.39	2.95	2.47	2.91	3.79	2.98	1.37	3.02	0.30	2.98	1.61	3.07	1.60	3.01	0.40	2.992	1.084
10	C6	337	0.69	3.271	3.34	2.10	3.30	0.99	3.28	0.42	3.27	0.00	3.24	0.99	3.39	3.58	3.35	2.52	3.23	1.41	3.227	1.357
11	C7	366	0.727	3.071	3.11	1.43	3.12	1.50	3.13	2.06	3.13	1.81	3.01	1.90	3.19	3.74	3.06	0.33	3.06	0.29	3.048	0.736
12	C8	390	0.749	2.877	2.88	0.17	2.91	1.11	2.95	2.43	2.98	3.41	2.81	2.47	2.96	2.93	2.82	1.93	2.89	0.28	2.869	0.271
13	C9	416	0.768	2.665	2.63	1.28	2.67	0.37	2.73	2.32	2.79	4.69	2.59	2.98	2.71	1.83	2.58	3.17	2.68	0.45	2.666	0.026
14	C10	439	0.782	2.481	2.42	2.35	2.47	0.30	2.53	2.04	2.61	5.36	2.40	3.30	2.51	0.99	2.39	3.80	2.49	0.48	2.486	0.218
15	C11	461	0.793	2.31	2.23	3.26	2.29	1.00	2.35	1.55	2.44	5.42	2.23	3.58	2.32	0.26	2.21	4.15	2.32	0.43	2.315	0.221
16	C12	482	0.804	2.165	2.08	3.86	2.13	1.56	2.19	1.12	2.28	5.16	2.08	3.92	2.16	0.15	2.07	4.18	2.17	0.32	2.171	0.259

Table 4. Cintinued

	Petroleum fraction	Input		Pc/MPa	Riazi and Daubert [12]		Riazi and Daubert [11]		Lee-Kesler Method [8]		Cavett Method [18]		Twu Method [20]		Winn Method [38]		Tsonopoulos et al. [37]		Mohammadi et al. [10]		New model	
		T_b/K	S	Exp.	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%
17	C13	501	0.815	2.054	1.96	4.36	2.01	2.10	2.07	0.68	2.15	4.55	1.96	4.47	2.04	0.47	1.97	4.11	2.05	0.10	2.059	0.234
18	C14	520	0.826	1.953	1.86	4.79	1.90	2.63	1.96	0.18	2.02	3.63	1.85	5.11	1.94	0.72	1.88	3.92	1.94	0.51	1.957	0.200
19	C15	539	0.836	1.853	1.76	5.03	1.80	3.02	1.85	0.31	1.90	2.55	1.75	5.65	1.84	0.79	1.79	3.48	1.84	0.76	1.857	0.227
20	C16	557	0.843	1.752	1.66	5.09	1.69	3.37	1.74	0.90	1.78	1.34	1.65	6.02	1.74	0.73	1.70	2.90	1.74	0.63	1.754	0.131
21	C17	573	0.851	1.679	1.59	5.18	1.62	3.67	1.66	1.42	1.68	0.12	1.57	6.58	1.67	0.69	1.64	2.37	1.67	0.77	1.681	0.095
22	C18	586	0.856	1.614	1.53	5.07	1.55	3.82	1.58	1.84	1.60	0.82	1.50	6.86	1.61	0.49	1.59	1.77	1.61	0.56	1.615	0.074
23	C19	598	0.861	1.559	1.48	4.95	1.50	3.94	1.52	2.23	1.53	1.71	1.45	7.17	1.55	0.27	1.54	1.17	1.55	0.45	1.560	0.083
24	C20	612	0.866	1.495	1.42	4.77	1.43	4.11	1.45	2.79	1.45	2.79	1.38	7.55	1.49	0.01	1.49	0.45	1.49	0.20	1.495	0.013
25	C21	624	0.871	1.446	1.38	4.60	1.39	4.20	1.40	3.22	1.39	3.69	1.33	7.92	1.45	0.26	1.45	0.23	1.44	0.14	1.446	0.014
26	C22	637	0.876	1.393	1.33	4.32	1.33	4.25	1.34	3.68	1.33	4.57	1.28	8.27	1.40	0.64	1.41	1.06	1.39	0.07	1.393	0.007
27	C23	648	0.881	1.356	1.30	4.27	1.30	4.40	1.30	4.21	1.28	5.46	1.24	8.77	1.37	0.77	1.38	1.61	1.36	0.07	1.355	0.074
28	C24	659	0.885	1.314	1.26	3.97	1.26	4.41	1.25	4.65	1.23	6.13	1.19	9.08	1.33	1.15	1.35	2.38	1.32	0.30	1.313	0.061
29	C25	671	0.888	1.263	1.22	3.43	1.21	4.33	1.20	5.11	1.18	6.62	1.15	9.28	1.29	1.77	1.31	3.40	1.27	0.63	1.263	0.040
30	C26	681	0.892	1.23	1.19	3.16	1.18	4.33	1.16	5.54	1.14	7.13	1.11	9.62	1.26	2.12	1.28	4.14	1.24	0.65	1.230	0.008
31	C27	691	0.896	1.2	1.16	3.03	1.15	4.43	1.13	6.10	1.11	7.72	1.08	10.09	1.23	2.33	1.26	4.74	1.21	0.50	1.199	0.125
32	C28	701	0.899	1.164	1.13	2.55	1.11	4.31	1.09	6.49	1.07	7.93	1.04	10.30	1.20	2.89	1.23	5.68	1.17	0.77	1.164	0.043
33	C29	709	0.902	1.14	1.11	2.32	1.09	4.31	1.06	6.89	1.05	8.20	1.02	10.61	1.18	3.18	1.21	6.30	1.15	0.79	1.139	0.053
34	C30	719	0.905	1.107	1.09	1.86	1.06	4.21	1.03	7.36	1.02	8.30	0.99	10.89	1.15	3.71	1.19	7.22	1.12	0.90	1.107	0.018
35	C31	728	0.909	1.085	1.07	1.71	1.04	4.22	1.00	7.86	0.99	8.55	0.96	11.32	1.13	3.94	1.17	7.85	1.09	0.65	1.085	0.046
36	C32	737	0.912	1.06	1.04	1.46	1.01	4.26	0.97	8.43	0.97	8.65	0.94	11.74	1.11	4.25	1.15	8.54	1.07	0.47	1.059	0.142
37	C33	745	0.915	1.039	1.03	1.20	1.00	4.21	0.95	8.86	0.95	8.62	0.91	12.05	1.09	4.58	1.13	9.22	1.04	0.29	1.038	0.144
38	C34	753	0.917	1.013	1.01	0.63	0.97	4.00	0.92	9.19	0.93	8.26	0.89	12.18	1.07	5.21	1.12	10.17	1.02	0.49	1.013	0.010
39	C35	760	0.92	0.998	0.99	0.52	0.96	4.02	0.90	9.64	0.92	8.22	0.87	12.56	1.05	5.38	1.10	10.67	1.00	0.20	0.997	0.070
40	C36	768	0.922	0.974	0.97	0.01	0.94	3.86	0.88	10.05	0.90	7.75	0.85	12.76	1.03	5.97	1.09	11.58	0.98	0.31	0.974	0.000
41	C37	774	0.925	0.964	0.96	0.02	0.93	3.90	0.86	10.48	0.89	7.71	0.84	13.14	1.02	6.00	1.08	11.93	0.96	0.21	0.963	0.104
42	C38	782	0.927	0.941	0.95	0.52	0.91	3.72	0.84	10.89	0.87	7.06	0.82	13.35	1.00	6.60	1.06	12.87	0.94	0.21	0.941	0.011
43	C39	788	0.929	0.927	0.93	0.74	0.89	3.67	0.82	11.27	0.87	6.66	0.80	13.61	0.99	6.88	1.05	13.43	0.92	0.32	0.927	0.032
44	C40	796	0.931	0.905	0.92	1.31	0.87	3.47	0.80	11.69	0.85	5.80	0.78	13.81	0.97	7.52	1.04	14.42	0.90	0.33	0.906	0.077
45	C41	801	0.933	0.896	0.91	1.37	0.86	3.50	0.79	12.10	0.85	5.49	0.77	14.14	0.96	7.61	1.03	14.75	0.89	0.67	0.896	0.033
46	C42	807	0.934	0.877	0.90	2.05	0.85	3.20	0.77	12.30	0.84	4.47	0.75	14.15	0.95	8.35	1.02	15.74	0.87	0.46	0.879	0.217
47	C43	813	0.936	0.864	0.88	2.33	0.84	3.10	0.75	12.69	0.83	3.76	0.74	14.40	0.94	8.68	1.01	16.37	0.86	0.69	0.866	0.220
48	C44	821	0.938	0.844	0.87	2.91	0.82	2.88	0.73	13.14	0.82	2.49	0.72	14.63	0.92	9.34	0.99	17.39	0.84	0.71	0.847	0.344
49	C45	826	0.94	0.835	0.86	3.09	0.81	2.80	0.72	13.47	0.82	1.83	0.71	14.87	0.91	9.54	0.98	17.88	0.83	0.96	0.838	0.323
				AARD%		**4.36**		**5.66**		**7.23**		**6.53**		**10.78**		**4.77**		**33.96**		**0.82**		**0.65**

[a]Quoted in Mohammadi et al. [10]

Table 5. Comparison of critical volume calculated by the new model with previous models for petroleum fractions

	Petroleum fraction	Input		$Vc/m^3 \cdot kmol^{-1}$	Riazi and Daubert [12]		Riazi and Daubert [11]		Twu method [20]		Mohammadi et al. [10]		New model	
		T_b/K^a	S^a	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	C1	112	0.3	0.099	0.103	4.45	0.002	97.76	0.093	5.80	0.094	5.1	0.099	0.00
2	C2	185	0.356	0.146	0.256	75.57	0.013	91.02	0.150	2.69	0.145	0.7	0.145	0.84
3	C3	231	0.507	0.2	0.240	19.99	0.130	35.12	0.201	0.57	0.203	1.5	0.204	1.79
4	i-C4	261	0.563	0.263	0.269	2.33	0.208	20.81	0.241	8.32	0.263	0	0.263	0.00
5	n-C4	273	0.584	0.255	0.282	10.45	0.240	6.04	0.258	1.07	0.277	8.6	0.269	5.52
6	i-C5	301	0.625	0.306	0.317	3.62	0.304	0.60	0.299	2.23	0.316	3.3	0.304	0.54
7	Ne-C5	283	0.597	0.304	0.296	2.73	0.261	14.04	0.273	10.33	0.293	3.6	0.281	7.53
8	N-C5	309	0.631	0.313	0.332	6.11	0.318	1.58	0.313	0.14	0.332	6.1	0.317	1.27
9	n-C6	342	0.664	0.371	0.388	4.64	0.382	2.95	0.369	0.57	0.389	4.9	0.371	0.01
10	C6	337	0.69	0.348	0.351	0.96	0.383	10.03	0.352	1.03	0.339	2.6	0.349	0.39
11	C7	366	0.727	0.392	0.392	0.07	0.430	9.61	0.399	1.90	0.376	4.1	0.391	0.33
12	C8	390	0.749	0.433	0.433	0.10	0.468	7.98	0.444	2.63	0.419	3.2	0.431	0.38
13	C9	416	0.768	0.484	0.485	0.13	0.512	5.72	0.498	2.96	0.473	2.3	0.481	0.52
14	C10	439	0.782	0.532	0.534	0.46	0.555	4.26	0.551	3.53	0.526	1.1	0.531	0.20
15	C11	461	0.793	0.584	0.587	0.44	0.601	2.83	0.606	3.71	0.58	0.7	0.583	0.10
16	C12	482	0.804	0.635	0.637	0.36	0.647	1.92	0.661	4.07	0.633	0.3	0.635	0.01
17	C13	501	0.815	0.681	0.683	0.29	0.691	1.51	0.712	4.62	0.679	0.3	0.681	0.04
18	C14	520	0.826	0.727	0.730	0.37	0.738	1.57	0.766	5.41	0.726	0.1	0.728	0.20
19	C15	539	0.836	0.777	0.779	0.24	0.790	1.71	0.824	6.00	0.775	0.3	0.778	0.16
20	C16	557	0.843	0.83	0.831	0.07	0.847	2.00	0.883	6.38	0.828	0.2	0.832	0.20
21	C17	573	0.851	0.874	0.875	0.06	0.898	2.73	0.936	7.05	0.872	0.2	0.876	0.23
22	C18	586	0.856	0.915	0.914	0.16	0.944	3.21	0.982	7.28	0.911	0.4	0.916	0.12
23	C19	598	0.861	0.951	0.949	0.17	0.989	4.01	1.025	7.75	0.948	0.3	0.953	0.17
24	C20	612	0.866	0.997	0.993	0.35	1.046	4.91	1.078	8.09	0.993	0.4	0.998	0.10
25	C21	624	0.871	1.034	1.030	0.34	1.096	6.03	1.123	8.61	1.031	0.3	1.035	0.14
26	C22	637	0.876	1.077	1.072	0.46	1.155	7.24	1.174	9.01	1.074	0.3	1.077	0.05
27	C23	648	0.881	1.11	1.106	0.36	1.206	8.66	1.217	9.61	1.109	0.1	1.111	0.08
28	C24	659	0.885	1.147	1.143	0.39	1.262	10.01	1.262	10.02	1.145	0.2	1.148	0.06
29	C25	671	0.888	1.193	1.186	0.59	1.328	11.34	1.315	10.23	1.193	0	1.193	0.00
30	C26	681	0.892	1.226	1.219	0.55	1.384	12.90	1.357	10.69	1.228	0.2	1.226	0.02
31	C27	691	0.896	1.259	1.253	0.49	1.443	14.60	1.400	11.17	1.263	0.3	1.259	0.04
32	C28	701	0.899	1.296	1.289	0.52	1.506	16.22	1.445	11.51	1.301	0.4	1.295	0.05
33	C29	709	0.902	1.323	1.317	0.44	1.558	17.78	1.481	11.91	1.33	0.5	1.323	0.04
34	C30	719	0.905	1.361	1.354	0.49	1.628	19.58	1.527	12.22	1.368	0.5	1.360	0.09
35	C31	728	0.909	1.389	1.385	0.31	1.691	21.72	1.567	12.78	1.398	0.6	1.388	0.10
36	C32	737	0.912	1.421	1.418	0.21	1.759	23.76	1.609	13.21	1.431	0.7	1.420	0.07
37	C33	745	0.915	1.448	1.447	0.08	1.821	25.77	1.646	13.66	1.459	0.8	1.447	0.06
38	C34	753	0.917	1.48	1.479	0.09	1.888	27.58	1.686	13.92	1.49	0.7	1.479	0.05
39	C35	760	0.92	1.502	1.503	0.09	1.947	29.61	1.718	14.37	1.513	0.7	1.501	0.06
40	C36	768	0.922	1.534	1.536	0.12	2.019	31.62	1.759	14.65	1.542	0.5	1.533	0.04
41	C37	774	0.925	1.55	1.556	0.39	2.073	33.72	1.785	15.17	1.56	0.6	1.550	0.02
42	C38	782	0.927	1.583	1.589	0.37	2.151	35.85	1.827	15.39	1.588	0.3	1.582	0.06
43	C39	788	0.929	1.604	1.612	0.51	2.210	37.79	1.857	15.74	1.607	0.2	1.604	0.03
44	C40	796	0.931	1.636	1.645	0.58	2.294	40.22	1.899	16.06	1.633	0.2	1.636	0.01
45	C41	801	0.933	1.652	1.664	0.74	2.347	42.06	1.923	16.39	1.648	0.2	1.652	0.01
46	C42	807	0.934	1.68	1.691	0.65	2.415	43.73	1.957	16.47	1.667	0.8	1.680	0.02
47	C43	813	0.936	1.701	1.715	0.82	2.483	45.97	1.987	16.83	1.684	1	1.701	0.02
48	C44	821	0.938	1.733	1.749	0.93	2.578	48.79	2.031	17.17	1.707	1.5	1.734	0.07
49	C45	826	0.94	1.749	1.768	1.10	2.639	50.90	2.055	17.50	1.74	0.5	1.750	0.05
				AARD%		**2.97**		**20.35**		**8.95**		**1.27**		**0.45**

[a]Quoted in Mohammadi et al. [10]

Table 6. Comparison of acentric factor calculated by the new model with previous models for petroleum fractions

	Petroleum fraction	Input		Acentric factor	Lee-Kesler method [35]		Edmister method [19]		Korsten method [36]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	C1	112	0.3	0.012	0.085	607.36	0.096	701.24	0.053	342.66	0.012	0	0.012	0.02
2	C2	185	0.356	0.1	0.141	40.71	0.149	49.37	0.125	25.36	0.1	0	0.100	0.00
3	C3	231	0.507	0.152	0.148	2.67	0.157	2.98	0.134	12.00	0.146	3.9	0.148	2.88
4	i-C4	261	0.563	0.177	0.188	6.04	0.197	11.17	0.178	0.44	0.187	5.6	0.185	4.27
5	n-C4	273	0.584	0.2	0.201	0.32	0.210	4.83	0.192	4.03	0.198	1	0.199	0.58
6	i-C5	301	0.625	0.228	0.234	2.70	0.243	6.40	0.228	0.06	0.228	0	0.235	2.94
7	Ne-C5	283	0.597	0.196	0.217	10.47	0.225	15.00	0.209	6.70	0.21	7.1	0.213	8.85
8	N-C5	309	0.631	0.252	0.251	0.42	0.259	2.79	0.246	2.38	0.242	4	0.249	1.12
9	n-C6	342	0.664	0.301	0.301	0.13	0.307	1.88	0.298	0.92	0.286	5	0.300	0.24
10	C6	337	0.69	0.251	0.247	1.43	0.255	1.58	0.243	3.39	0.249	0.8	0.257	2.54
11	C7	366	0.727	0.28	0.273	2.37	0.280	0.08	0.270	3.55	0.278	0.7	0.282	0.67
12	C8	390	0.749	0.312	0.303	2.93	0.308	1.37	0.301	3.56	0.311	0.3	0.311	0.31
13	C9	416	0.768	0.352	0.339	3.57	0.342	2.85	0.339	3.79	0.353	0.3	0.349	0.82
14	C10	439	0.782	0.389	0.375	3.61	0.375	3.62	0.375	3.62	0.392	0.8	0.388	0.38
15	C11	461	0.793	0.429	0.412	3.88	0.409	4.61	0.413	3.81	0.433	0.9	0.429	0.10
16	C12	482	0.804	0.467	0.447	4.18	0.441	5.54	0.448	4.12	0.472	1.1	0.468	0.29
17	C13	501	0.815	0.501	0.478	4.69	0.468	6.55	0.478	4.67	0.506	1	0.501	0.00
18	C14	520	0.826	0.536	0.508	5.32	0.495	7.64	0.507	5.38	0.54	0.7	0.533	0.49
19	C15	539	0.836	0.571	0.539	5.56	0.523	8.35	0.538	5.73	0.576	0.9	0.568	0.45
20	C16	557	0.843	0.61	0.574	5.90	0.554	9.16	0.572	6.20	0.614	0.7	0.610	0.08
21	C17	573	0.851	0.643	0.602	6.43	0.579	10.02	0.599	6.84	0.646	0.5	0.641	0.36
22	C18	586	0.856	0.672	0.627	6.67	0.601	10.56	0.624	7.18	0.675	0.4	0.671	0.11
23	C19	598	0.861	0.698	0.650	6.87	0.621	11.02	0.646	7.48	0.701	0.4	0.698	0.06
24	C20	612	0.866	0.732	0.679	7.30	0.646	11.74	0.673	8.03	0.733	0.1	0.734	0.21
25	C21	624	0.871	0.759	0.702	7.57	0.666	12.23	0.695	8.39	0.761	0.3	0.761	0.27
26	C22	637	0.876	0.789	0.727	7.81	0.689	12.71	0.720	8.73	0.791	0.3	0.793	0.47
27	C23	648	0.881	0.815	0.747	8.28	0.706	13.35	0.739	9.28	0.816	0.1	0.816	0.13
28	C24	659	0.885	0.841	0.770	8.46	0.726	13.72	0.761	9.54	0.842	0.1	0.844	0.34
29	C25	671	0.888	0.874	0.798	8.74	0.750	14.21	0.787	9.93	0.876	0.2	0.881	0.82
30	C26	681	0.892	0.897	0.817	8.91	0.767	14.53	0.806	10.17	0.9	0.3	0.905	0.86
31	C27	691	0.896	0.944	1.032	9.33	0.783	17.01	0.824	12.68	0.925	2	0.928	1.70
32	C28	701	0.899	0.968	1.056	9.12	0.802	17.11	0.845	12.69	0.951	1.8	0.957	1.16
33	C29	709	0.902	0.985	1.074	9.04	0.816	17.14	0.860	12.66	0.971	1.4	0.976	0.92
34	C30	719	0.905	1.008	1.098	8.90	0.835	17.16	0.881	12.60	0.998	1	1.005	0.34
35	C31	728	0.909	1.026	1.116	8.74	0.849	17.26	0.896	12.65	1.019	0.7	1.021	0.50
36	C32	737	0.912	1.046	1.136	8.58	0.865	17.31	0.914	12.63	1.041	0.5	1.043	0.25
37	C33	745	0.915	1.063	1.153	8.43	0.878	17.37	0.929	12.64	1.061	0.2	1.060	0.26
38	C34	753	0.917	1.082	1.172	8.29	0.894	17.36	0.946	12.57	1.081	0.1	1.085	0.27
39	C35	760	0.92	1.095	1.185	8.23	0.905	17.38	0.958	12.54	1.097	0.2	1.095	0.02
40	C36	768	0.922	1.114	1.204	8.06	0.920	17.39	0.975	12.49	1.117	0.3	1.119	0.43
41	C37	774	0.925	1.124	1.214	8.00	0.928	17.43	0.983	12.51	1.129	0.4	1.121	0.30
42	C38	782	0.927	1.142	1.232	7.91	0.943	17.38	1.000	12.40	1.148	0.5	1.143	0.12
43	C39	788	0.929	1.154	1.245	7.85	0.954	17.36	1.012	12.34	1.161	0.6	1.154	0.00
44	C40	796	0.931	1.172	1.263	7.73	0.969	17.34	1.028	12.26	1.178	0.5	1.175	0.30
45	C41	801	0.933	1.181	1.272	7.69	0.976	17.34	1.036	12.24	1.188	0.6	1.178	0.21
46	C42	807	0.934	1.195	1.286	7.64	0.989	17.26	1.050	12.11	1.201	0.5	1.200	0.45
47	C43	813	0.936	1.207	1.298	7.56	0.999	17.27	1.061	12.09	1.212	0.4	1.208	0.06
48	C44	821	0.938	1.224	1.316	7.48	1.013	17.22	1.077	11.98	1.227	0.2	1.226	0.16
49	C45	826	0.94	1.232	1.324	7.49	1.020	17.19	1.085	11.93	1.235	0.2	1.224	0.63
				AARD%		**19.33**		**26.52**		**15.59**		**1.012**		**0.79**

[a]Quoted in Mohammadi et al. [10]

Table 7. Comparison of critical temperature calculated by the new model with previous models for normal paraffins

	Normal paraffin	Input		Tc/K	Riazi and Daubert [12]		Riazi and Daubert [11]		Lee-Kesler method [8]		Cavett method [18]		Twu method [20]		Winn method [38]		Tsonopoulos et al. [37]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	n-Heptane	371.58	0.688	540	542.25	0.42	540.43	0.08	539.87	0.02	538.51	0.28	540.33	0.06	537.53	0.46	539.26	0.14	543.00	0.60	540.34	0.06
2	n-Octane	398.83	0.707	569	570.87	0.33	570.01	0.18	568.38	0.11	567.45	0.27	569.70	0.12	565.51	0.61	567.61	0.24	573.00	0.70	569.31	0.05
3	n-Nonane	423.97	0.722	595	596.27	0.21	596.16	0.19	593.52	0.25	593.67	0.22	595.76	0.13	590.54	0.75	593.07	0.32	599.00	0.70	595.04	0.01
4	n-Docane	447.3	0.734	618	619.02	0.16	619.48	0.24	615.91	0.34	617.42	0.09	619.04	0.17	613.15	0.79	616.09	0.31	623.00	0.80	618.11	0.02
5	n-Undecene	469.08	0.745	639	640.00	0.16	640.86	0.29	636.40	0.41	639.38	0.06	640.41	0.22	634.09	0.77	637.40	0.25	644.00	0.80	639.36	0.06
6	n-Dodecane	489.47	0.753	658	658.75	0.11	659.88	0.28	654.64	0.51	659.09	0.17	659.41	0.21	652.97	0.76	656.62	0.21	664.00	0.90	658.42	0.06
7	n-Tridecane	508.62	0.762	675	676.68	0.25	677.96	0.44	672.00	0.44	677.88	0.43	677.48	0.37	671.04	0.59	674.99	0.00	683.00	1.20	676.55	0.23
8	n-Tetradecane	526.73	0.763	693	691.09	0.28	692.30	0.10	685.84	1.03	693.20	0.03	691.91	0.16	685.87	1.03	690.07	0.42	699.00	0.90	691.56	0.21
9	n-Pentadecane	543.83	0.772	708	707.18	0.12	708.39	0.05	701.32	0.94	709.97	0.28	707.96	0.01	702.16	0.82	706.58	0.20	715.00	1.00	707.71	0.04
10	n-Hexadecane	560.01	0.777	723	721.16	0.26	722.22	0.11	714.70	1.15	724.65	0.23	721.83	0.16	716.49	0.90	721.08	0.27	730.00	1.00	721.98	0.14
11	n-Heptadecane	575.3	0.78	736	733.70	0.31	734.48	0.21	726.64	1.27	737.90	0.26	734.23	0.24	729.44	0.89	734.16	0.25	743.00	1.00	734.94	0.14
12	n-Octadecane	589.86	0.782	747	745.25	0.23	745.65	0.18	737.60	1.26	750.21	0.43	745.62	0.18	741.45	0.74	746.26	0.10	756.00	1.20	747.00	0.00
13	n-Nonadecane	603.05	0.787	758	756.75	0.17	756.90	0.15	748.57	1.24	762.23	0.56	756.89	0.15	753.29	0.62	758.20	0.03	767.00	1.20	758.64	0.08
14	n-Eicosane	616.93	0.792	768	768.70	0.09	768.54	0.07	759.96	1.05	774.74	0.88	768.57	0.07	765.64	0.31	770.65	0.34	780.00	1.60	770.75	0.36
15	n-Heicosane	629.7	0.795	782	779.08	0.37	778.50	0.45	769.81	1.56	785.75	0.48	778.70	0.42	776.46	0.71	781.52	0.06	791.00	1.20	781.45	0.07
16	n-Docosane	641.8	0.798	792	788.92	0.39	787.91	0.52	779.14	1.62	796.20	0.53	788.27	0.47	786.74	0.66	791.83	0.02	801.00	1.10	791.58	0.05
17	n-Tricosane	653.4	0.8	801	798.00	0.37	796.47	0.57	787.72	1.66	805.97	0.62	797.10	0.49	796.27	0.59	801.37	0.05	810.00	1.10	801.04	0.01
18	n-Tetracosane	664.4	0.803	810	806.97	0.37	805.00	0.62	796.23	1.70	815.51	0.68	805.78	0.52	805.65	0.54	810.77	0.10	819.00	1.10	810.23	0.03
				AARD%		**0.26**		**0.26**		**0.92**		**0.36**		**0.23**		**0.70**		**0.18**		**1.01**		**0.09**

[a]Quoted in Mohammadi et al. [10]

Table 8. Comparison of critical pressure calculated by the new model with previous models for normal paraffins

	Normal paraffin	Input		Pc/Mpa	Riazi and Daubert [12]		Riazi and Daubert [11]		Lee-Kesler method [8]		Cavett method [18]		Twu method [20]		Winn method [38]		Tsonopoulos et al. [37]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	n-Heptane	371.58	0.688	2.74	2.647	3.41	2.676	2.35	2.654	3.15	2.723	0.63	2.738	0.06	2.682	2.11	2.704	1.32	2.78	1.46	2.717	0.82
2	n-Octane	398.83	0.707	2.49	2.394	3.87	2.434	2.25	2.425	2.60	2.507	0.69	2.503	0.51	2.436	2.17	2.424	2.67	2.564	2.97	2.481	0.35
3	n-Nonane	423.97	0.722	2.29	2.182	4.72	2.222	2.95	2.221	3.00	2.315	1.09	2.299	0.40	2.227	2.73	2.201	3.87	2.371	3.50	2.277	0.58
4	n-Docane	447.3	0.734	2.11	2.003	5.08	2.037	3.45	2.040	3.33	2.140	1.41	2.121	0.53	2.050	2.86	2.020	4.26	2.202	4.40	2.098	0.56
5	n-Undecene	469.08	0.745	1.949	1.857	4.70	1.883	3.39	1.887	3.17	1.988	2.01	1.968	0.99	1.905	2.26	1.875	3.81	2.054	5.40	1.947	0.09
6	n-Dodecane	489.47	0.753	1.82	1.726	5.19	1.740	4.40	1.742	4.26	1.841	1.18	1.829	0.48	1.773	2.61	1.746	4.07	1.923	5.70	1.810	0.58
7	n-Tridecane	508.62	0.762	1.68	1.623	3.39	1.627	3.13	1.629	3.05	1.723	2.58	1.711	1.87	1.670	0.58	1.646	2.04	1.815	8.00	1.698	1.06
8	n-Tetradecane	526.73	0.763	1.57	1.502	4.36	1.490	5.08	1.483	5.54	1.576	0.36	1.587	1.11	1.545	1.58	1.530	2.55	1.701	8.30	1.573	0.20
9	n-Pentadecane	543.83	0.772	1.48	1.433	3.18	1.413	4.51	1.405	5.05	1.492	0.81	1.498	1.24	1.477	0.18	1.463	1.15	1.623	9.70	1.494	0.92
10	n-Hexadecane	560.01	0.777	1.4	1.359	2.91	1.329	5.09	1.317	5.95	1.400	0.01	1.410	0.73	1.403	0.19	1.392	0.57	1.545	10.40	1.413	0.91
11	n-Heptadecane	575.3	0.78	1.34	1.289	3.83	1.247	6.94	1.229	8.25	1.311	2.13	1.327	0.94	1.330	0.72	1.324	1.18	1.471	9.80	1.338	0.19
12	n-Octadecane	589.86	0.782	1.27	1.224	3.66	1.171	7.80	1.147	9.65	1.230	3.12	1.251	1.50	1.264	0.51	1.262	0.66	1.404	10.60	1.270	0.02
13	n-Nonadecane	603.05	0.787	1.21	1.180	2.49	1.120	7.42	1.094	9.60	1.175	2.86	1.192	1.48	1.220	0.79	1.220	0.79	1.353	11.80	1.221	0.87
14	n-Eicosane	616.93	0.792	1.16	1.136	2.08	1.069	7.84	1.040	10.39	1.120	3.42	1.133	2.35	1.175	1.31	1.177	1.49	1.303	12.30	1.172	0.99
15	n-Heicosane	629.7	0.795	1.147	1.093	4.72	1.019	11.20	0.985	14.14	1.068	6.90	1.077	6.09	1.131	1.37	1.136	0.97	1.254	9.30	1.127	1.78
16	n-Docosane	641.8	0.798	1.101	1.055	4.18	0.974	11.54	0.937	14.94	1.022	7.15	1.027	6.69	1.093	0.75	1.099	0.15	1.209	9.80	1.087	1.24
17	n-Tricosane	653.4	0.8	1.059	1.018	3.86	0.930	12.17	0.889	16.08	0.979	7.53	0.980	7.48	1.055	0.40	1.064	0.44	1.167	10.20	1.051	0.74
18	n-Tetracosane	664.4	0.803	1.019	0.988	3.03	0.895	12.19	0.850	16.56	0.945	7.31	0.939	7.87	1.024	0.51	1.035	1.55	1.128	10.70	1.021	0.17
				AARD%		**3.81**		**6.32**		**7.71**		**2.84**		**2.35**		**1.31**		**1.86**		**8.02**		**0.67**

[a]Quoted in Mohammadi et al. [10]

tal data of pure hydrocarbons has been excluded from training set.

Modeling based on GP starts with selecting terminals and functions sets. As an example, Fig. 1 shows (C×exp (A−(A×B))) expression in the tree structure format. In the tree structure, functions and terminals are combined with specific grammar. In this structure, the terminals and functions set are placed in external and internal nodes, respectively. A, B and C are the terminals set, while ×, − and exponential function are the functions set. Mathematical functions such as (+, −, /, ×, ^, ln, exp) have been selected as function set (FS) in this work. Terminals set involves input variables (normal boiling point and specific gravity, TS=(T_b, S)). The maximum and minimum values of terminals set (input variable) for training and testing are reported in Table 1. After identifying the terminals and functions sets, the adjustable parameters of GP (population, generation size, fraction and type of each genetic operator) must be specified. The population of each generation can be thousands or millions; however, it should be considered that computation time and the need for advanced computing systems sharply increases as the population size increases. Therefore, choosing an optimum population size increases the convergence time. The optimum population size is dependent on the type and difficulty of modeling. In this work, we aimed at generation of a simple as well as highly accurate model, so based on our previous experiences, population and generation size have been set to 25000 and 2000, respectively. Meanwhile, the main genetic operators such as selection, mutation, and crossover have been applied to generate new models. Roulette wheel approach has been considered as a selection operator. Many authors have suggested that the crossover operator must be between 70-90 percent of the individuals of population size. Therefore, the crossover, reproduction and mutation operator probability have been performed on 87%, 8% and 5%, respectively.

RESULTS

The mentioned approach was used to model critical properties and acentric factor of petroleum fractions. We used different functions for modeling of critical properties and acentric factor. Modeling was carried out in two steps: preliminary and final modeling. In the preliminary step of modeling, all adequate mathematical functions were used as function set. The results of this step showed that mathematical functions such as (+, −, /, ×, ^, ln, exp) can be included in the final models. Therefore, choosing the appropriate functions from the preliminary modeling results saved the time in the modeling of final step. In GP approach, results are generated based on stochastic optimization method. In each iteration, a new model is produced; however, most of the results are similar. The technical information of genetic programming structure is reported in Table 2. Reported values in Table 2 are the optimum ones which led us to achieve the efficient models. The following results were obtained after 2000 generations. The obtained models for acentric factor, critical temperature, pressure and volume are presented in Eqs. (1)-(4):

$$T_C = 853.7359\left(\frac{S^4\sqrt{S}}{\exp(S)}\right) + 430.4936\left(\frac{S}{T_b} + \sqrt{S}\right) + 1.6340\left(\frac{T_b}{\sqrt[4]{S}\exp(S)}\right) - 232.3511 \quad (1)$$

.

$$P_C = 0.0412265T_b + 54.8996S - 32.0724\ln(T_bS + 37.66) + 13.2269\ln(T_b) - 8.03833\times10^{-3}\frac{S^2\ln(2S)(T_b - S)}{\exp(S)} + 58.253 \quad (2)$$

Table 9. Comparison of critical volume calculated by the new model with previous models for normal paraffins

	Normal paraffin	Input		Vc/m^3·kmol^{-1}	Riazi and Daubert [12]		Riazi and Daubert [11]		Twu Method [20]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	n-Heptane	371.58	0.688	0.428	0.446	4.12	0.438	2.26	0.425	0.69	0.447	4.40	0.427	0.34
2	n-Octane	398.83	0.707	0.486	0.504	3.67	0.490	0.88	0.482	0.80	0.507	4.30	0.484	0.48
3	n-Nonane	423.97	0.722	0.544	0.563	3.42	0.541	0.50	0.540	0.75	0.567	4.20	0.542	0.42
4	n-Docane	447.3	0.734	0.6	0.622	3.62	0.592	1.39	0.598	0.27	0.627	4.50	0.600	0.06
5	n-Undecene	469.08	0.745	0.659	0.679	3.05	0.642	2.55	0.657	0.29	0.685	3.90	0.658	0.10
6	n-Dodecane	489.47	0.753	0.716	0.738	3.09	0.693	3.23	0.717	0.08	0.743	3.80	0.717	0.15
7	n-Tridecane	508.62	0.762	0.775	0.793	2.30	0.744	4.00	0.775	0.05	0.797	2.80	0.774	0.18
8	n-Tetradecane	526.73	0.763	0.83	0.860	3.60	0.795	4.17	0.837	0.87	0.862	3.90	0.836	0.67
9	n-Pentadecane	543.83	0.772	0.889	0.910	2.33	0.848	4.62	0.896	0.73	0.911	2.50	0.889	0.04
10	n-Hexadecane	560.01	0.777	0.944	0.965	2.23	0.901	4.60	0.955	1.14	0.966	2.30	0.945	0.11
11	n-Heptadecane	575.3	0.78	1	1.022	2.24	0.953	4.69	1.014	1.42	1.024	2.40	1.001	0.09
12	n-Octadecane	589.86	0.782	1.06	1.080	1.93	1.006	5.13	1.073	1.27	1.081	2.00	1.057	0.33
13	n-Nonadecane	603.05	0.787	1.12	1.127	0.60	1.057	5.63	1.128	0.69	1.127	0.60	1.105	1.34
14	n-Eicosane	616.93	0.792	1.17	1.177	0.59	1.114	4.78	1.187	1.46	1.176	0.50	1.158	1.07
15	n-Heicosane	629.7	0.795	1.198	1.228	2.50	1.169	2.44	1.244	3.87	1.227	2.40	1.209	0.88
16	n-Docosane	641.8	0.798	1.253	1.277	1.90	1.223	2.36	1.300	3.77	1.275	1.80	1.258	0.38
17	n-Tricosane	653.4	0.8	1.307	1.327	1.52	1.278	2.24	1.356	3.74	1.323	1.20	1.307	0.01
18	n-Tetracosane	664.4	0.803	1.362	1.372	0.74	1.333	2.16	1.409	3.49	1.368	0.40	1.353	0.66
				AARD%		**2.41**		**3.20**		**1.41**		**2.66**		**0.41**

[a]Quoted in Mohammadi et al. [10]

Table 10. Comparison of acentric factor calculated by the new model with previous models for normal paraffins

	Normal paraffin	Input		Acentric factor	Lee-Kesler method [35]		Edmister method [19]		Korsten method [36]		Mohammadi et al. [10]		New model	
		T_b/K[a]	S[a]	Exp.[a]	Cal.	ARD%	Cal.	ARD%	Cal.	ARD%	Cal.[a]	ARD%[a]	Cal.	ARD%
1	n-Heptane	371.580	0.688	0.350	0.348	0.62	0.351	0.32	0.347	0.86	0.332	5.10	0.350	0.08
2	n-Octane	398.830	0.707	0.400	0.393	1.70	0.393	1.71	0.393	1.71	0.378	5.50	0.398	0.56
3	n-Nonane	423.970	0.722	0.444	0.438	1.36	0.434	2.23	0.438	1.33	0.423	4.70	0.445	0.17
4	n-Docane	447.300	0.734	0.492	0.482	1.94	0.474	3.58	0.482	1.96	0.467	5.10	0.491	0.23
5	n-Undecene	469.080	0.745	0.530	0.524	1.11	0.512	3.45	0.523	1.26	0.510	3.80	0.535	0.87
6	n-Dodecane	489.470	0.753	0.576	0.568	1.36	0.551	4.34	0.566	1.67	0.553	4.00	0.579	0.50
7	n-Tridecane	508.620	0.762	0.617	0.606	1.72	0.585	5.23	0.603	2.19	0.592	4.10	0.619	0.39
8	n-Tetradecane	526.730	0.763	0.643	0.661	2.81	0.633	1.54	0.656	2.06	0.640	0.50	0.667	3.66
9	n-Pentadecane	543.830	0.772	0.686	0.693	1.08	0.661	3.60	0.687	0.20	0.675	1.60	0.703	2.52
10	n-Hexadecane	560.010	0.777	0.717	0.733	2.27	0.696	2.92	0.726	1.19	0.714	0.40	0.742	3.53
11	n-Heptadecane	575.300	0.780	0.770	0.776	0.78	0.733	4.76	0.766	0.48	0.756	1.80	0.781	1.46
12	n-Octadecane	589.860	0.782	0.811	0.820	1.08	0.771	4.88	0.808	0.37	0.797	1.70	0.819	1.03
13	n-Nonadecane	603.050	0.787	0.852	0.851	0.11	0.799	6.27	0.838	1.67	0.830	2.60	0.852	0.01
14	n-Eicosane	616.930	0.792	0.907	1.008	11.16	0.828	8.71	0.870	4.07	0.864	4.70	0.888	2.15
15	n-Heicosane	629.700	0.795	0.922	1.045	13.33	0.859	6.79	0.905	1.90	0.900	2.40	0.922	0.03
16	n-Docosane	641.800	0.798	0.955	1.079	13.00	0.889	6.90	0.937	1.88	0.934	2.20	0.955	0.04
17	n-Tricosane	653.400	0.800	0.989	1.113	12.57	0.920	6.95	0.971	1.80	0.967	2.20	0.987	0.22
18	n-Tetracosane	664.400	0.803	1.019	1.144	12.22	0.947	7.04	1.001	1.79	0.999	2.00	1.018	0.14
				AARD%		**4.46**		**4.51**		**1.58**		**3.02**		**0.98**

[a]Quoted in Mohammadi et al. [10]

$$V_C = 0.28652S + 2.942\times10^{-4}T_bS\sqrt{T_bS} - 2.563\times10^{-3}T_b^S - 4.7768 \times10^{-3}T_bS^2 + 3.8254\times10^{-6}\left(\frac{T_b+2S-\exp(S)}{\ln S+2S^2}\right) + 0.014865 \quad (3)$$

$$\omega = 5.46505\times10^{-3}T_b - 0.4708(\ln(1-S^2))^2 + 4.1183 \times10^{-6}S^8(T_b+S)^2 - 1.58018\sqrt{S} - 7.3528\times10^{-5}\left(\frac{T_b\sqrt{T_b}}{S}\right) + 0.56011 \quad (4)$$

T_b and S represent boiling point and specific gravity, respectively. The units of T_C, P_C and V_C are in Kelvin, MPa and m^3/kmol, respectively.

To check the capability of the obtained models, the results have been compared with previous models in Tables 3 to 6. Relative absolute deviation (ARD) and average absolute relative deviation (AARD) have been selected as objective function in this work (Eqs. (5) and (6)). These functions also were used for performance evaluation of each model. The obtained AARD for predicting critical temperature, pressure, volume and acentric of petroleum fractions were equal to 0.07, 0.65, 0.45 and 0.79, respectively. It can be seen that the new correlations have higher accuracy compared to the previous works.

$$ARD\% = \sum\left|\frac{Q^{exp}-Q^{cal}}{Q^{exp}}\right|\times100 \quad (5)$$

$$AARD\% = \frac{1}{N}\sum_1^N\left|\frac{Q^{exp}-Q^{cal}}{Q^{exp}}\right|\times100 \quad (6)$$

Q represents properties of petroleum fractions.

To validate the new model, critical properties of normal paraffins have been predicted. The results of the new models in prediction of critical temperature and pressure, and critical volume and acentric factor of pure hydrocarbons are shown in Tables 7 to 10. AARD percent of the test data set in prediction of critical temperature, pressure, and volume and acentric factor were equal to 0.09, 0.67, 0.41 and 0.98, respectively. Twu method [20] was used for calculation of the required input parameters of acentric factor

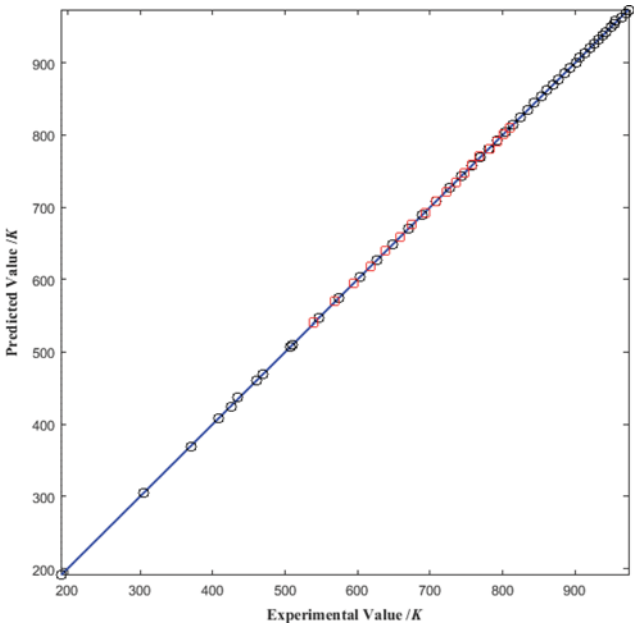

Fig. 2. Calculated and predicted critical temperature using new model versus the experimental values, ○: petroleum fractions, □: normal paraffins.

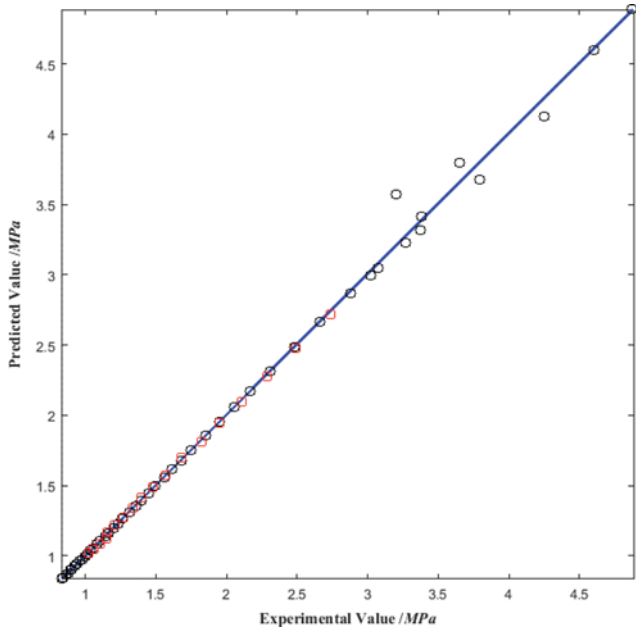

Fig. 3. Calculated and predicted critical pressure using new model versus the experimental values, ○: petroleum fractions, □: normal paraffins.

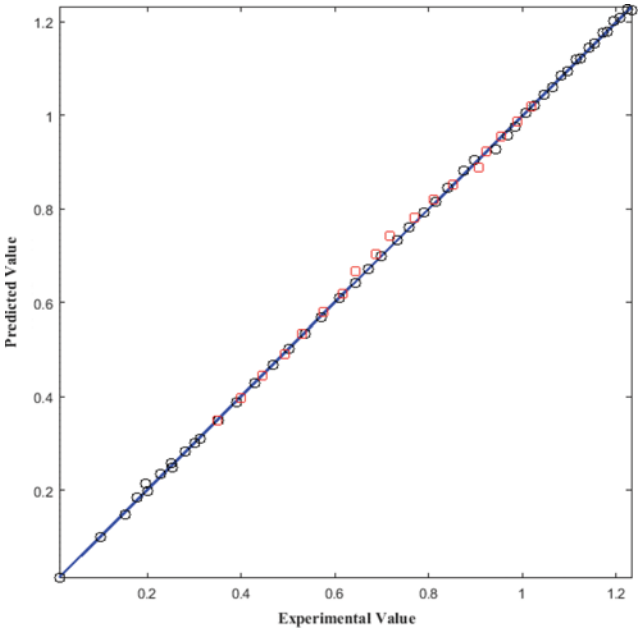

Fig. 5. Calculated and predicted acentric factor using new model versus the experimental values, ○: petroleum fractions, □: normal paraffins.

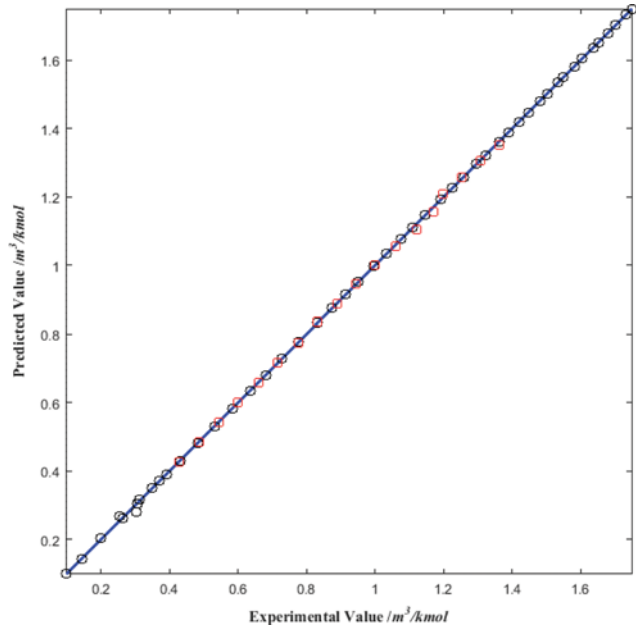

Fig. 4. Calculated and predicted critical volume using new model versus the experimental values, ○: petroleum fractions, □: normal paraffins.

by Lee-Kesler [35], Edmister [19] and Korsten methods [36]. Figs. 2-5 show the predicted value versus experimental data for each property of petroleum fractions and normal paraffins (training and testing data set). A good agreement between predicted and experimental data proves new models can predict the critical properties and acentric factor of hydrocarbons with high accuracy. Note that the experimental data of normal paraffins were excluded from training sets.

CONCLUSIONS

This study demonstrated that the genetic programming approach can be used for modeling of experimental data. Considering the strong demand for accurate correlations in calculation of critical properties and acentric factor of petroleum fractions (especially, heavy petroleum fractions), in this work new correlations have been developed for prediction of critical temperature, pressure, and volume and acentric factor of petroleum fraction using genetic programming as a function of average normal boiling points and specific gravities values. Our results showed that new correlations can be used efficiently for prediction of critical properties.

NOMENCLATURE

AARD% : average absolute relative deviations
ARD% : absolute relative deviations
ANN : artificial neural network
FS : function set
GP : genetic programming
GC : group contribution
M : molecular weight
N : number of experimental data
OLS : orthogonal least squares
P : pressure
QSPR : quantitative structure property relationship
S : specific gravity
T : temperature
TS : terminals set

V : volume

Greek Symbols

ω : acentric factor

Subscripts

b : normal boiling point
c : critical

Superscript

exp : experimental
cal : calculated

REFERENCES

1. T. Hatami, M. Rahimi, H. Daraei, E. Heidaryan and A. A. Alsairafi, *Korean J. Chem. Eng.*, **29**, 657 (2012).
2. J.-N. Jaubert and F. Mutelet, *Fluid Phase Equilib.*, **224**, 285 (2004).
3. J.-N. Jaubert, R. Privat and F. Mutelet, *AIChE J.*, **56**, 3225 (2010).
4. A. Shariati, S.-S. Ashrafmansouri, M. H. Osbuei and B. Hooshdaran, *Korean J. Chem. Eng.*, **30**, 187 (2013).
5. S. Vitu, R. Privat, J.-N. Jaubert and F. Mutelet, *J. Supercrit. Fluids*, **45**, 1 (2008).
6. A. Danesh, *Pvt and phase behaviour of petroleum reservoir fluids*, Elsevier (1998).
7. F. Gharagheizi, A. Eslamimanesh, A. H. Mohammadi and D. Richon, *J. Chem. Eng. Data*, **56**, 2460 (2011).
8. M. G. Kesler and B. I. Lee, *Hydrocarbon Processing*, **55**, 153 (1976).
9. G. M. Kontogeorgis, I. Smirlis, I. V. Yakoumis, V. Harismiadis and D. P. Tassios, *Ind. Eng. Chem. Res.*, **36**, 4008 (1997).
10. A. H. Mohammadi, W. Afzal and D. Richon, D., *Ind. Eng. Chem. Res.*, **47**, 3225 (2008).
11. M. R. Riazi and T. E. Daubert, *Ind. Eng. Chem. Res.*, **26**, 755 (1987).
12. M. R. Riazi and T. E. Daubert, *Hydrocarbon Processing*, **59**, 115 (1980).
13. R. Riazi, *Characterization and properties of petroleum fractions*, American Society for Testing & Materials (2005).
14. Q. Wang, Q. Jia and P. Ma, *J. Chem. Eng. Data*, **57**, 169 (2011).
15. P. He and A. F. Ghoniem, *Ind. Eng. Chem. Res.*, **54**, 8809 (2015).
16. X. Xu, J.-N. Jaubert, R. Privat, P. Duchet-Suchaux and F. Braña-Mulero, *Ind. Eng. Chem. Res.*, **54**, 2816 (2015).
17. A. Mohammadi, M. Omidkhah, R. Karimzadeh and A. Haghtalab, *Korean J. Chem. Eng.*, **30**, 465 (2012).
18. R. Cavett, Physical data for distillation calculations, vapour-liquid equilibria, *Proc. of 27th API Meeting*, San Francisco, 351 (1962).
19. W. C. Edmister, *Pet. Refiner*, **37**, 173 (1958).
20. C. H. Twu, *Fluid Phase Equilib.*, **16**, 137 (1984).
21. H. Cao, J. Yu, L. Kang and Y. Chen, *Comput. Chem.*, **23**, 143 (1999).
22. B. McKay, M. Willis and G. Barton, *Comput. Chem. Eng.*, **21**, 981 (1997).
23. E. M. E.-M. Shokir, *Energy Fuels*, **22**, 3194 (2008).
24. X.-H. Wang, Y.-D. Hu and Y.-G. Li, *Korean J. Chem. Eng.*, **25**, 402 (2008).
25. E. M. E.-M. Shokir, M. N. El-Awad, A. A. Al-Quraishi and O. A. Al-Mahdy, *Chem. Eng. Res. Design*, **90**, 785 (2012).
26. E. M. E.-M. Shokir and H. N. Dmour, *Energy Fuels*, **23**, 3632 (2009).
27. A. A. AlQuraishi, *Energy Fuels*, **23**, 884 (2009).
28. H. Parhizgar, M. R. Dehghani and A. Eftekhari, *J. Petroleum Sci. Eng.*, **112**, 97 (2013).
29. J. R. Koza, *Genetic programming: On the programming of computers by means of natural selection*, MIT Press (1992).
30. W. Banzhaf, *Genetic programming: An introduction on the automatic evolution of computer programs and its applications*, Morgan Kaufmann Publishers (1998).
31. J. R. Koza, *Genetic programming iii: Darwinian invention and problem solving*, Morgan Kaufmann (1999).
32. J. R. Koza, M. A. Keane, M. J. Streeter, W. Mydlowec, J. Yu and G. Lanza, *Genetic programming iv: Routine human-competitive machine intelligence*, Springer (2005).
33. H. F. Costa, H. l. Lourenço, I. Johnson, F. A.M. M. Gonçalves, A. G. M. Ferreira and I. M. A. Fonseca, *J. Chem. Eng. Data*, **54**, 2845 (2009).
34. R. Riolo, T. McConaghy and E. Vladislavleva, *Genetic programming theory and practice viii*, Springer (2010).
35. B. I. Lee and M. G. Kesler, *AIChE J.*, **21**, 510 (1975).
36. H. Korsten, *Ind. Eng. Chem. Res.*, **39**, 813 (2000).
37. C. Tsonopoulos, J. L. Heidman and S. Hwang, *Thermodynamic and transport properties of coal liquids*, John Wiley and Sons, New York, NY, United States (1986).
38. F. Winn, *Petroleum Refiner*, **36**, 157 (1957).