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An Efficient Method for Correlation of Vapor Pressure of Gaseous Compounds Containing C-H-O

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Prediction of available vapor pressure data in the case of compounds containing C-H-O led to derivations and recommendations of standard equations for this property. The accuracy of vapor pressure estimations is essential to use as a basis to calculate acentric factor, thermal and equilibrium properties. In this study, according to the previous work, an accurate equation to estimate vapor pressure is developed to 130 pure C-H-O compounds as a function of reduced temperature and critical pressure. With new proposed equation, vapor pressures have been calculated in comparison with experimental data reported in literature for 2019 data points of 130 pure C-H-O compounds and the overall average absolute relative deviation is only 0.333%. The accuracy of the developed equation has been compared to that of Antoine and other mostly used equations. Our comparisons show that new equation leads to more accurate results than those of literature methods.

Keywords: Vapor pressure, C-H-O, Pure compounds, Correlation, Antoine

INTRODUCTION

Reliable liquid vapor pressure prediction is essential to develop equations of state to simulate, evaluate and optimize chemical processes. The accuracy of vapor pressure calculations is very important because of using as a basis to calculate acentric factor, thermal and equilibrium properties [1]. Authentic vapor pressure data are important in process design equipment. Most oil and gas processing operations such as oil refinery requires vapor pressure data for estimation of phase equilibrium. The vapor pressure or equilibrium vapor pressure is a good indication of liquid evaporation rate in combustion modeling. In numerical simulations, significant changes in the fuel atomization and evaporation rates lead to change in fuel vapor pressure [2].

Because of absence and limited range of vapor pressure experimental data in the literature, some researchers have used different vapor pressure correlations to estimate parameters in equations of state [3-7].

Numerous empirical vapor pressure equations have been published until now. The best known are those of Wagner [8], Clausius, Antoine, Frost-Kalkwarf, Cox, Gomez-Thodos, Lee-Kesler, Ambrose-Walton, Riedel [9,10] and Lemmon-Goodwin [11]. The most common of all vapor pressure correlations is Antoine [12] with three constant parameters, which is valid only within a limited temperature range. In this work we extend the previous equation [13] to 130 pure mostly used C-H-O compounds which are formed with only C, H and O elements. Based on this model, a predictive correlation is developed. The source of saturated vapor pressure experimental data used in this study is Ref. [14].

VAPOR PRESSURE CORRELATION MODELS

Antoine Correlation

The Antoine vapor pressure correlation was modified

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based on Clapeyron equation. It is widely used to estimate vapor pressures over limited temperature range [12]. The Antoine correlation is shown below:

$$\ln P_{vp} = A - \frac{B}{T + C} \tag{1}$$

where P_{vp} is the vapor pressure (*mmHg*), T is the temperature (°*C*) and the constant values of *A*, *B* and *C* for some species are presented in Appendix A in [9].

Lee-Kesler's Method

Lee-Kesler equation [9] is one of the successful methods to predict vapor pressure using six-parameter formulations.

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \tag{2}$$

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.28862 \ln T_r + 0.169347 T_r^6 \tag{3}$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.4721 \ln T_r + 0.43577 T_r^6 \tag{4}$$

Where P_{vpr} is the reduced vapor pressure which is equal to P/P_c. P_c is the critical pressure (*pascal*), ω is the acentric factor, T_r is the reduced temperature which is equal to T/T_c, and T_c is the critical temperature (*K*) of the fluid. Values for T_c and P_c can be found in the literature for many pure substances [10,15].

Ambrose-Walton Corresponding States Method

Ambrose and Walton [10] developed another representation of the Pitzer expansion with an additional term $f^{(2)}(T_r)$.

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) + \omega^2 f^{(2)}(T_r) \tag{5}$$

$$f^{(0)} = \frac{-5.97616\tau + 1.29874\tau^{1.5} - 0.60394\tau^{2.5} - 1.06841\tau^5}{T_r} \tag{6}$$

$$f^{(1)} = \frac{-5.03365\tau + 1.11505\tau^{1.5} - 5.41217\tau^{2.5} - 7.46628\tau^5}{T_r} \tag{7}$$

$$f^{(2)} = \frac{-0.64771\tau + 2.41539\tau^{1.5} - 4.26979\tau^{2.5} + 3.25259\tau^5}{T_r} \tag{8}$$

$$\omega = -\frac{\ln(P_c/1.01325) + f^{(0)}(T_{br})}{f^{(1)}(T_{br})} \tag{9}$$

Where ω is the acentric factor, P_c is the critical pressure (*bars*) of the fluid, and $\tau = 1\text{-}T_r$.

Riedel Correlation Method

Riedel [16] proposed a vapor pressure equation in following form:

$$\ln P_{vpr} = A + \frac{B}{T_r} + C \ln T_r + D T_r^6 \tag{10}$$

the T_r^6 term allows description of the inflection point of the vapor pressure curve in the high-pressure region. Parameters *A*, *B*, *C* and *D* are functions of T, T_c, T_b and P_c.

Wagner Equation

Wagner [8] used an elaborate statistical method to present an equation for representing the vapor pressure behavior of nitrogen and argon over the wide temperature range. The resulting equation is:

$$\ln\left(\frac{P_{sat}}{P_c}\right) = \frac{A\tau + B\tau^{1.5} + C\tau^{2.5} + D\tau^5}{1 - \tau} \tag{11}$$

where $\tau = 1 - T/T_c$, P_c is the critical pressure and T_c is the critical temperature.

Luis *et al.* [1] determined Wagner equation parameters for 257 substances with low deviations. However, there are a few joint substances with the present work for a correct comparison with Wagner [8] and Luis [1] work.

Sanjari Equation

Sanjari [13] tried to find a new simple equation for the vapor pressure of pure substances. It is a four-constant non-linear correlation that reproduces vapor-liquid equilibrium data with high accuracy even at low reduced temperatures. Sanjari [13] empirical correlation was presented as follow:

$$\ln P_{vpr} = a + \frac{b}{T_r} + c \ln T_r + d T_r^2 \tag{12}$$

where P_{vpr} is reduced vapor pressure which is equal to P/P_c, $T_r = T/T_c$ is the reduced temperature, and the coefficients *a*,

b, *c* and *d* are constant parameters.

DEVELOPED EQUATION

This work tries to develop a new model to estimate vapor pressure of pure C-H-O compounds by the help of vapor pressure experimental data more accurate than other models in terms of reduced temperature and critical pressure. There are many available data in sources [14] to allow the proposition of a model for vapor pressure of pure substances. After multiple regression analysis, the coefficients *A*, *B*, *C* and *D* are constant parameters and their values for 130 C-H-O substances are presented in Table 1. Also for more information about obtained constant parameters, (R^2) of each substance in fitting procedure is presented in Table 1.

The obtained equation presented in this study is:

$$\ln P_{vpr} = A + \frac{B}{T_r} + C T_r + B T_r^{1.9} \tag{13}$$

Also Table 1 shows the number of data points, critical temperatures, critical pressures, and temperature ranges of experimental data for each substance.

RESULT AND DISCUSSION

We carried out calculations for 130 pure C-H-O

Table 1. Critical Properties, Temperature Range, and Tuned Coefficients to be Used in Eq. (13)

	Name	Formula	No of data	T_{min}	T_{max}	T_c (K)	P_c (bar)	*A*	*B*	*C*	*D*	R^2
1	Methane	CH_4	19	92.2	126.5	190.6	45.99	6.194	-4.791	2.287	-1.770	0.9999
2	Methanol	CH_4O	59	288.0	307.3	512.6	80.97	10.480	-8.620	2.048	-2.120	1
3	Acetylene	C_2H_2	27	192.6	206.3	308.3	61.38	10.144	-23.343	-37.848	14.216	1
4	Ketene	C_2H_2O	10	185.4	223.8	370.0	58.10	29.282	89.015	258.332	-138.313	1
5	Ethylene	C_2H_4	26	123.5	188.6	282.3	50.41	7.153	-8.766	-5.805	1.628	0.9999
6	Ethylene oxide-1	C_2H_4O	29	223.8	305.0	469.2	71.90	8.159	-12.356	-12.604	4.579	0.9999
7	Acetic acid	$C_2H_4O_2$	18	303.0	399.6	592.0	57.86	10.464	-17.219	-20.340	7.158	1
8	Ethane	C_2H_6	33	135.7	199.9	305.3	48.72	6.793	-9.405	-7.673	2.832	0.9998
9	Dimethyl ether	C_2H_6O	11	194.9	248.2	400.1	53.70	8.778	-9.727	-5.507	0.768	1
10	Ethanol	C_2H_6O	31	273.2	366.6	513.9	61.48	12.783	-12.081	-3.029	-0.797	1
11	Ethylene glycol	$C_2H_6O_2$	31	323.2	473.2	720.0	82.00	14.511	-17.592	-15.724	3.083	0.9999
12	Propyne	C_3H_4	31	161.6	254.3	402.4	56.30	8.142	-6.167	3.025	-2.034	1
13	Cyclopropane	C_3H_6	13	183.1	241.1	397.9	54.95	8.299	-7.487	-1.137	-1.284	0.9999
14	Propylene	C_3H_6	12	165.8	226.0	364.9	46.00	7.974	-9.573	-6.454	1.573	1
15	1-Propen-3-ol	C_3H_6O	6	294.2	370.2	545.1	56.20	8.901	74.808	207.609	-92.656	1
16	Acetone-1	C_3H_6O	8	310.8	329.2	508.2	47.02	10.651	-23.859	-37.590	14.350	1
17	Acetone-2	C_3H_6O	15	260.2	328.4	508.2	47.02	9.791	-11.902	-8.904	2.092	0.9999
18	Propylene oxide	C_3H_6O	6	249.0	307.9	482.3	49.20	8.663	-20.191	-30.873	12.868	0.9999
19	Ethyl formate	$C_3H_6O_2$	13	277.0	326.7	508.4	47.42	10.460	-16.032	-18.428	5.997	0.9999
20	Methyl acetate	$C_3H_6O_2$	15	274.9	329.0	506.6	47.50	10.846	-10.195	-3.289	-1.076	1
21	Propanoic acid-1	$C_3H_6O_2$	13	329.7	401.5	600.8	46.17	33.898	401.502	1042.786	-488.724	0.9996
22	Propane	C_3H_8	12	166.0	231.4	369.8	42.48	8.305	-8.035	-2.244	-0.603	0.9999

Table 1. Continued

23	1-Propanol	C_3H_8O	19	333.3	377.7	536.8	51.75	14.901	-14.368	-6.194	-0.644	1
24	2-Propanol	C_3H_8O	17	325.5	362.4	508.3	47.64	15.696	-15.566	-7.862	-0.197	1
25	Methyl ethyl ether	C_3H_8O	5	278.2	280.9	437.8	44.00	-154.15	-1.406	-156.452	202.070	0.9967
26	Ethyleneglycol monomethyl ether	$C_3H_8O_2$	19	329.3	396.7	564.0	50.10	8.656	2.348	27.943	-12.297	0.9999
27	Methylal	$C_3H_8O_2$	8	273.2	308.2	480.6	39.52	10.539	12.562	52.390	-26.208	0.9999
28	Glycerol	$C_3H_8O_3$	20	456.4	533.6	850.0	75.00	25.580	36.894	131.011	-71.951	0.9997
29	2-Methylpropane	C_4H_{10}	9	188.1	261.5	407.8	36.40	8.611	-9.391	-4.963	0.607	1
30	Butane	C_4H_{10}	11	195.1	272.8	425.1	37.96	8.575	-10.806	-8.368	2.272	1
31	2-Butanol	$C_4H_{10}O$	16	345.5	380.3	538.2	42.19	18.180	-20.322	-17.514	2.092	1
32	Diethyl ether	$C_4H_{10}O$	17	212.4	293.0	466.7	36.40	10.039	-12.409	-10.023	2.350	1
33	Isobuatol	$C_4H_{10}O$	16	353.4	388.8	547.8	43.00	17.615	-19.136	-15.015	1.440	1
34	Methyl propyl ether	$C_4H_{10}O$	26	272.6	312.5	476.3	38.01	-25.025	429.443	1047.258	-445.512	0.9886
35	Tert-butanol	$C_4H_{10}O$	14	333.9	362.7	506.2	39.73	21.593	-27.649	-31.402	6.105	0.9999
36	2-Ethoxyethanol	$C_4H_{10}O_2$	13	336.2	407.2	569.0	42.40	11.131	-12.768	-6.555	1.473	0.9999
37	Diethylene glycol	$C_4H_{10}O_3$	25	403.2	516.2	744.6	46.00	21.353	-80.597	-163.449	64.865	0.9999
38	Diacetylene	C_4H_2	14	195.0	273.2	478.0	58.63	27.235	-8.355	13.458	-29.218	0.9998
39	Diacetylene	C_4H_2	8	199.6	234.0	478.0	58.63	222.903	201.670	703.191	-579.689	0.9999
40	Furan	C_4H_4O	13	275.7	334.6	490.2	55.00	9.263	-11.452	-9.070	2.224	1
41	1,2-Butadiene	C_4H_6	12	197.7	271.7	425.4	43.30	8.816	-9.450	-4.862	0.396	0.9999
42	1,3-Butadiene	C_4H_6	4	191.3	249.2	425.4	43.30	33.545	58.221	186.212	-110.576	1
43	1-Butyne	C_4H_6	17	194.4	282.7	443.2	49.50	9.728	-9.743	-4.116	-0.335	1
44	Cyclobutene	C_4H_6	12	196.1	275.1	446.3	52.66	3.494	-19.517	-35.062	19.053	0.9999
45	Vinyl acetate	$C_4H_6O_2$	12	295.0	345.2	519.1	39.58	10.659	-15.820	-17.128	5.554	0.9999
46	Acetic anhydride	$C_4H_6O_3$	22	336.0	412.6	606.0	40.00	12.669	-19.308	-22.874	7.000	0.9999
47	1-Butene	C_4H_8	21	195.7	269.5	419.6	40.20	9.409	6.245	34.493	-18.060	0.9992
48	2-Methylpropene	C_4H_8	7	216.4	273.2	417.9	39.99	8.581	-18.771	-28.232	11.048	0.9999
49	Cis-2-butene	C_4H_8	17	203.1	295.9	435.6	42.06	8.822	-11.331	-9.352	2.576	1
50	Cyclobutane	C_4H_8	12	213.2	285.3	459.9	49.80	8.054	-9.827	-6.720	1.745	1
51	Trans-2-butene	C_4H_8	11	201.7	274.1	428.6	41.02	8.451	-11.130	-9.217	2.775	1
52	Butyraldehyde	C_4H_8O	9	303.9	347.2	537.2	43.20	12.017	30.822	98.864	-48.704	0.9999
53	Isobutyraldehyde	C_4H_8O	10	286.1	336.0	507.0	41.00	11.060	-12.528	-8.845	1.056	0.9999
54	Methyl ethyl ketone	C_4H_8O	17	315.9	361.6	535.5	41.54	10.199	-12.017	-8.524	1.780	1
55	Tetrahydrofurane	C_4H_8O	15	296.3	372.9	540.2	51.88	9.132	-11.153	-8.371	2.030	1
56	1,4-Dioxane	$C_4H_8O_2$	11	293.2	378.2	587.0	52.08	9.029	-9.343	-3.441	0.323	0.9999
57	Butyric acid	$C_4H_8O_2$	8	364.1	436.4	615.7	40.64	17.899	-35.425	-55.172	18.708	1
58	Ethyl acetate	$C_4H_8O_2$	16	288.7	349.0	523.3	38.80	11.201	-14.378	-12.874	3.276	1
59	Methyl propionate	$C_4H_8O_2$	15	293.7	351.9	530.6	40.04	11.676	-22.425	-32.464	11.616	0.9999

Table 1. Continued

60	Propyl formate	$C_4H_8O_2$	16	299.4	355.5	538.0	40.63	9.388	31.513	98.492	-45.589	0.9997
60	Propyl formate	$C_4H_8O_2$	16	299.4	355.5	538.0	40.63	9.388	31.513	98.492	-45.589	0.9997
61	1-Pentene	C_5H_{10}	8	286.0	303.9	464.8	35.60	6.658	11.674	45.614	-20.265	1
62	2-Methyl-1-butene	C_5H_{10}	13	274.3	335.8	465.0	34.00	9.403	-11.464	-8.728	2.105	1
63	2-Methyl-2-butene	C_5H_{10}	14	277.2	343.7	470.0	34.20	12.278	-22.139	-31.789	10.302	0.9999
64	3-Methyl-1-butene	C_5H_{10}	11	273.4	324.3	452.7	35.30	8.679	-9.930	-5.975	1.208	1
65	Cis-2-pentene	C_5H_{10}	14	274.7	342.0	475.9	36.54	9.308	-10.930	-7.478	1.598	1
66	Cyclopentane	C_5H_{10}	11	288.9	323.2	511.7	45.10	8.691	-8.556	-2.688	-0.375	1
67	Trans-2-pentene	C_5H_{10}	14	274.2	341.4	475.4	36.54	9.157	-10.593	-6.819	1.417	1
68	Diethyl ketone	$C_5H_{10}O$	17	329.7	384.5	560.9	37.40	10.843	-13.114	-10.308	2.260	0.9999
69	Methyl propyl ketone	$C_5H_{10}O$	18	329.8	384.8	561.1	36.94	10.985	-13.714	-11.677	2.733	0.9996
70	Butyl formate	$C_5H_{10}O_2$	19	302.3	385.6	559.0	35.10	9.380	-8.013	1.244	-1.341	0.9999
71	Ethyl propanoate	$C_5H_{10}O_2$	16	306.9	371.5	546.0	33.62	12.130	-16.160	-16.045	4.145	1
72	Propyl acetate	$C_5H_{10}O_2$	15	312.2	374.0	549.7	33.60	12.123	-17.737	-19.975	5.907	1
73	Sec butyl formate	$C_5H_{10}O_2$	16	302.9	373.0	546.0	35.80	15.331	-125.01	-282.665	121.299	0.9995
74	Iso pentane	C_5H_{12}	7	289.4	301.7	460.4	33.80	8.461	-6.957	1.295	-1.817	1
75	Neopentane	C_5H_{12}	15	231.2	282.6	433.8	31.96	4.606	-7.775	-5.189	3.904	0.9998
76	Pentane	C_5H_{12}	9	286.4	310.0	469.7	33.70	9.120	-9.269	-3.510	-0.030	1
77	1-Pentanol	$C_5H_{12}O$	19	347.9	429.1	588.1	38.97	17.902	-18.720	-13.780	0.599	1
78	2-Pentanol	$C_5H_{12}O$	10	298.1	383.3	560.3	36.75	19.220	-24.520	-26.800	5.413	0.9999
79	Ethyl propyl ether	$C_5H_{12}O$	15	293.5	335.7	500.2	33.70	9.374	-3.961	10.589	-6.157	0.9999
80	Methyl butyl ether	$C_5H_{12}O$	18	296.1	342.1	512.7	33.71	9.956	-7.344	2.716	-3.129	0.9999
81	Diethoxymethane	$C_5H_{12}O_2$	16	273.2	348.2	524.0	32.80	10.965	-14.938	-14.389	3.935	0.9999
82	Propyl cellosive	$C_5H_{12}O_2$	8	350.3	421.9	615.2	36.51	14.992	-27.217	-39.545	13.091	0.9999
83	Isoperene	C_5H_8	12	256.9	306.4	484.0	38.50	9.151	-6.660	2.431	-2.954	1
84	Spiropentane	C_5H_8	14	279.8	344.0	499.7	52.13	13.073	-42.184	-81.335	31.396	0.9998
85	2,3-Dimethyl-1,3-butadien	C_6H_{10}	9	273.2	341.6	526.0	35.20	9.366	-7.046	2.191	-2.657	0.9999
86	3-Hexyne	C_6H_{10}	21	253.2	297.6	544.0	35.30	9.834	17.955	64.819	-30.959	0.9995
87	1-Hexene	C_6H_{12}	13	289.0	337.5	504.0	32.10	9.750	-10.975	-6.760	1.117	1
88	2,3-Dimethyl-2-butene	C_6H_{12}	9	302.2	346.4	528.0	33.20	9.814	-11.186	-7.430	1.433	1
89	3,3-Dimethyl-1-butene	C_6H_{12}	16	263.7	314.7	480.0	32.90	9.092	-10.329	-6.404	1.136	1
90	Cyclohexane-1	C_6H_{12}	17	293.1	354.7	553.8	40.80	9.249	-10.439	-6.590	1.078	0.9993
91	Cyclohexane-2	C_6H_{12}	5	279.5	294.1	553.8	40.80	-144.57	-339.40	-962.417	598.050	1
92	Cyclohexanol	$C_6H_{12}O$	16	366.9	433.9	650.1	42.60	19.078	-3.649	22.998	-18.117	0.9999
93	Butyl acetate	$C_6H_{12}O_2$	15	332.9	399.2	575.4	30.90	12.350	-18.316	-20.811	6.278	0.9999
94	2,2-Dimethyl butane	C_6H_{14}	11	288.5	323.7	489.0	31.00	9.054	-9.589	-4.534	0.377	1
95	2,3-Dimethyl butane	C_6H_{14}	13	287.4	331.9	500.0	31.50	9.264	-10.662	-6.828	1.333	1

Table 1. Continued

96	2-Methyl pentane	C_6H_{14}	14	285.9	334.2	497.7	30.40	9.567	-10.130	-4.906	0.417	1
97	2-Methyl pentane	C_6H_{14}	13	288.4	337.2	504.4	31.24	9.538	-10.871	-6.841	1.265	1
98	Hexane	C_6H_{14}	16	286.2	342.7	507.6	30.25	10.069	-12.293	-9.543	2.236	1
99	1-Hexanol	$C_6H_{14}O$	13	325.4	430.5	610.3	34.17	20.021	-27.337	-32.894	7.502	0.9999
100	2-Hexanol	$C_6H_{14}O$	14	298.2	415.2	585.9	33.10	16.962	-18.219	-13.751	1.177	0.9999
101	2-Methyl-1-pentanol	$C_6H_{14}O$	13	298.2	418.2	604.4	34.50	14.651	-8.919	6.469	-6.273	0.9999
102	2-Methyl-4-pentanol	$C_6H_{14}O$	13	423.2	406.2	604.4	34.50	-5.135	99.704	255.113	-101.817	0.9997
103	3-Hexanol	$C_6H_{14}O$	13	298.2	411.2	579.3	33.10	10.862	4.685	36.147	-16.836	0.9999
104	DiIsopropyl ether	$C_6H_{14}O$	19	296.7	340.4	500.1	28.80	11.860	-22.185	-31.822	11.028	0.9999
105	Dipropyle ether	$C_6H_{14}O$	22	299.7	361.8	530.6	30.28	10.828	-14.290	-13.176	3.543	0.9999
106	Ethyl butyl ether	$C_6H_{14}O$	20	311.3	364.5	531.0	29.90	11.177	-15.278	-15.103	4.213	0.9999
107	Benzene	C_6H_6	19	287.7	354.1	562.1	48.95	9.273	-12.057	-10.562	2.855	1
108	Phenol	C_6H_6O	6	380.3	454.9	694.3	61.30	13.300	-20.817	-26.005	7.857	1
109	Resorcinol	$C_6H_6O_2$	18	424.7	549.7	810.0	74.90	15.409	-5.758	15.613	-11.227	0.999361
110	Pyrogallol	$C_6H_6O_3$	19	473.4	582.2	830.0	88.10	-37.723	303.780	728.207	-287.737	0.9971
111	1,1-Dimethylcyclopentane	C_7H_{14}	18	288.6	361.9	547.0	34.45	9.547	-11.221	-7.815	1.567	1
112	1-heptene	C_7H_{14}	17	294.8	367.7	537.3	29.20	10.480	-12.557	-9.440	2.037	1
113	Cis-1,2-dimethylcyclopentane	C_7H_{14}	20	296.5	373.6	565.2	34.45	9.402	3.316	28.068	-14.420	0.9999
114	Cis-1,3-dimethylcyclopentane	C_7H_{14}	18	299.1	365.8	551.0	34.45	9.618	-11.750	-8.953	2.073	1
115	Cycloheptane	C_7H_{14}	15	341.4	432.2	604.2	38.20	9.493	-11.575	-8.891	2.074	1
116	Ethylcyclopentane	C_7H_{14}	20	301.9	377.5	569.5	34.00	9.720	-11.881	-9.147	2.170	1
117	Methylcyclohexane	C_7H_{14}	20	298.7	375.0	572.1	34.80	9.340	-11.596	-9.143	2.276	1
118	trans-1,2-Dimethylcyclopentane	C_7H_{14}	18	299.3	365.9	553.2	34.45	9.608	-12.801	-11.627	3.286	1
119	Trans-1,3-dimethylcyclopentane	C_7H_{14}	19	291.2	364.8	553.0	34.45	9.543	-11.738	-9.131	2.185	1
120	2,4-Dimethyl-3-pentanone	$C_7H_{14}O$	8	321.2	398.4	576.0	30.20	10.531	-7.905	2.629	-3.192	1
121	Butyl propanoate	$C_7H_{14}O_2$	11	305.6	366.1	594.6	28.00	-0.264	-67.436	-153.661	79.966	0.9992
122	Heptanoic acid	$C_7H_{14}O_2$	20	385.8	422.7	677.3	30.43	29.157	-278.87	-644.471	277.287	
123	2,2-Dimethylpentane	C_7H_{16}	17	288.5	353.2	520.5	27.70	9.818	-10.578	-5.665	0.631	1
124	2,3-Dimethylpentane	C_7H_{16}	20	290.7	363.8	537.3	29.10	10.272	-16.307	-19.319	6.427	9999
125	2,4-Dimethylpentane	C_7H_{16}	13	286.9	340.4	519.8	27.40	10.209	-11.441	-7.245	1.123	1
126	2-Methylhexane	C_7H_{16}	18	291.7	363.0	530.4	27.40	10.520	-12.308	-8.828	1.737	1
127	3-Ethylpentane	C_7H_{16}	15	294.3	365.9	540.6	28.90	10.321	-12.095	-8.675	1.727	1
128	3-Methylhexane	C_7H_{16}	15	293.1	363.8	535.2	28.10	19.328	13.122	62.693	-38.855	0.9987
129	Heptane	C_7H_{16}	19	299.1	372.4	540.2	27.40	10.904	-13.543	-11.294	2.665	1
130	Toluene	C_7H_8	20	308.5	384.7	591.8	41.08	9.883	-8.093	0.319	-2.305	0.9999

compounds. The values of the vapor pressure, temperature, critical pressure, critical temperature, boiling point, and acentric factor, (used for calculation of literature models) were taken from data bank [15].

To compare the accuracy of the presented empirical model, calculated vapor pressures for all substances versus corresponded values of experimental data are presented in Fig. 1.

In Table 2, average absolute relative deviation (AARD%) of the calculated vapor pressure from proposed model and literature methods for all 130 substances with respect to the values given by experimental data are presented. It shows that new presented model is more

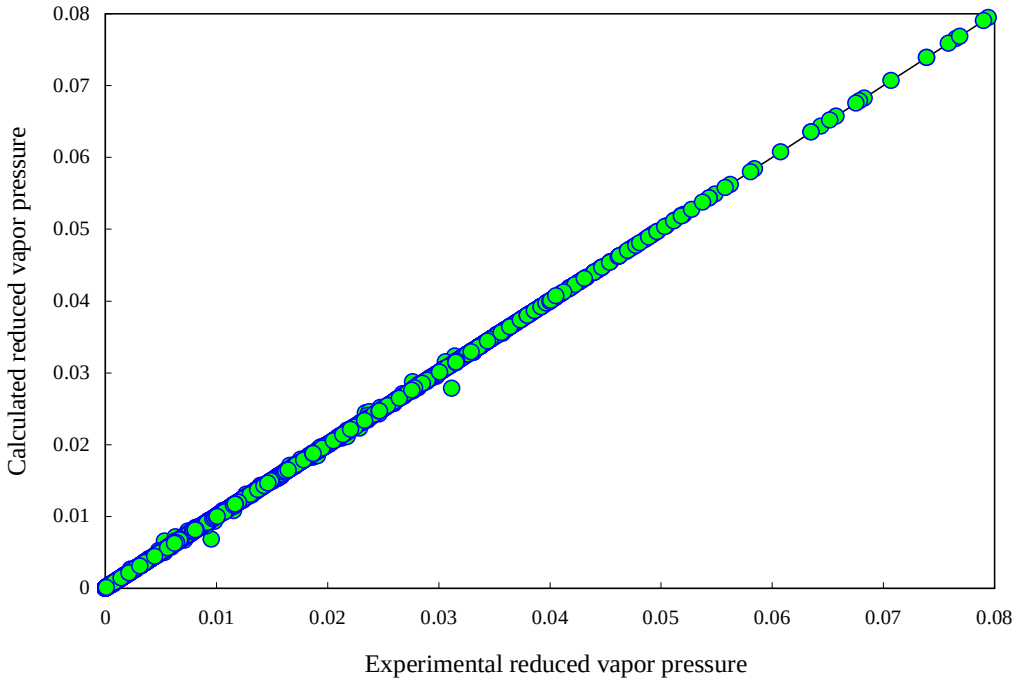

Fig. 1. Accuracy of presented model *vs.* experimental data.

Table 2. Average Absolute Relative Deviation of Four Literature Equations Compared to New Method

Name	Formula	Lee kesler	Antoine	Ambrose	Riedel	This study
Methane	CH_4	2.557	0.061	0.472	0.896	0.375
Methanol	CH_4O	12.803	0.075	10.740	8.736	0.096
Acetylene	C_2H_2	1.096	0.056	0.069	4.151	0.033
Ketene	C_2H_2O	7.757	1.070	10.666	2.468	0.434
Ethylene	C_2H_4	0.580	2.391	2.013	0.595	0.052
Ethylene oxide-1	C_2H_4O	1.197	0.099	1.425	0.780	0.326
Acetic acid	$C_2H_4O_2$	13.951	0.147	12.166	7.816	0.076

Table 2. Continued

Ethane	C_2H_6	2.926	0.213	0.778	0.881	0.198
Dimethyl ether	C_2H_6O	3.595	0.045	0.330	1.162	0.022
Ethanol	C_2H_6O	3.034	0.078	1.855	1.721	0.019
Ethylene glycol	$C_2H_6O_2$	15.006	0.116	18.783	10.372	1.178
Propyne	C_3H_4	5.024	0.354	4.339	4.261	0.716
Cyclopropane	C_3H_6	2.027	0.143	1.513	0.582	0.102
Propylene	C_3H_6	1.551	0.109	2.292	0.610	0.079
1-Propen-3-ol	C_3H_6O	7.884	0.525	5.370	6.673	0.106
Acetone	C_3H_6O	2.669	0.011	1.189	1.469	0.010
Propylene oxide	C_3H_6O	5.986	0.153	3.223	1.933	0.066
Ethyl formate	$C_3H_6O_2$	1.527	0.054	1.528	0.793	0.052
Methyl acetate	$C_3H_6O_2$	3.913	0.053	1.168	1.244	0.039
Propanoic acid-1	$C_3H_6O_2$	4.391	1.332	2.557	2.663	1.065
Propane	C_3H_8	2.825	0.137	0.556	1.522	0.079
1-Propanol	C_3H_8O	1.531	0.015	2.075	1.628	0.005
2-Propanol	C_3H_8O	1.256	0.011	1.582	1.771	0.003
Methyl ethyl ether	C_3H_8O	3.490	0.191	4.646	2.255	0.138
Ethyleneglycol monomethyl ether	$C_3H_8O_2$	11.725	0.293	11.164	11.899	0.265
Methylal	$C_3H_8O_2$	0.497	0.138	1.848	1.309	0.101
Glycerol	$C_3H_8O_3$	13.406	3.258	16.029	5.636	1.957
2-Methylpropane	C_4H_{10}	2.066	0.113	0.781	1.072	0.032
Butane	C_4H_{10}	2.876	0.174	0.220	1.232	0.142
2-Butanol	$C_4H_{10}O$	6.586	0.009	6.219	25.834	0.004
Diethyl ether	$C_4H_{10}O$	2.287	0.275	1.876	0.489	0.180
Isobuatol	$C_4H_{10}O$	3.527	0.008	3.881	2.930	0.003
Methyl propyl ether	$C_4H_{10}O$	3.639	1.971	2.117	2.452	0.491
tert-Butanol	$C_4H_{10}O$	2.372	0.069	2.653	2.458	0.096
2-Ethoxyethanol	$C_4H_{10}O_2$	7.274	0.418	6.843	9.855	0.447
Diethylene glycol	$C_4H_{10}O_3$	6.552	2.803	8.178	8.408	0.850
Diacetylene	C_4H_2	4.207	7.480	5.030	4.859	3.117
Diacetylene	C_4H_2	12.051	2.572	17.956	18.135	1.361
Furan	C_4H_4O	1.314	0.004	2.969	0.384	0.004
1,3-Butadiene	C_4H_6	3.966	0.313	0.961	1.692	0.303
1,3-Butadiene	C_4H_6	6.267	1.099	3.143	3.456	0.000
1-Butyne	C_4H_6	3.604	0.304	0.279	1.039	0.059
Cyclobutene	C_4H_6	8.147	0.908	5.499	2.503	0.488
Vinyl acetate	$C_4H_6O_2$	0.823	0.059	1.381	0.453	0.063
Acetic anhydride	$C_4H_6O_3$	5.351	0.102	3.786	4.525	0.101
1-Butene	C_4H_8	1.741	2.127	1.233	1.839	0.864

Table 2. Continued

2-Methylpropene	C_4H_8	1.362	0.204	1.244	1.531	0.199
Cis-2-butene	C_4H_8	1.849	0.037	0.799	0.408	0.027
Cyclobutane	C_4H_8	8.396	0.117	4.780	3.705	0.098
Trans-2-butene	C_4H_8	6.979	0.126	3.923	3.165	0.121
Butyraldehyde	C_4H_8O	1.997	0.276	0.340	0.347	0.085
Isobutyraldehyde	C_4H_8O	6.812	0.078	4.935	4.943	0.076
Methyl ethyl ketone	C_4H_8O	1.049	0.006	0.310	0.737	0.004
Tetrahydrofurane	C_4H_8O	1.677	0.007	0.243	3.885	0.004
1,4-Dioxane	$C_4H_8O_2$	3.396	0.064	0.724	1.371	0.034
Butyric acid	$C_4H_8O_2$	4.049	0.194	2.871	1.603	0.297
Ethyl acetate	$C_4H_8O_2$	2.164	0.023	0.305	0.468	0.023
Methyl propionate	$C_4H_8O_2$	1.568	0.083	0.938	0.431	0.048
Propyl formate	$C_4H_8O_2$	2.914	0.513	1.470	1.002	0.716
1-Pentene	C_5H_{10}	1.142	0.007	0.084	0.207	0.006
2-Methyl-1-butene	C_5H_{10}	0.170	0.383	1.120	0.264	0.026
2-Methyl-2-butene	C_5H_{10}	1.962	0.009	1.134	1.199	0.409
3-Methyl-1-butene	C_5H_{10}	0.906	0.002	0.147	0.328	0.002
Cis-2-pentene	C_5H_{10}	0.904	0.001	0.318	0.261	0.003
Cyclopentane	C_5H_{10}	1.322	0.007	0.555	0.214	0.006
Trans-2-pentene	C_5H_{10}	0.502	0.003	0.678	0.191	0.004
Diethyl ketone	$C_5H_{10}O$	0.551	0.026	1.225	0.528	0.002
Methyl propyl ketone	$C_5H_{10}O$	0.590	0.891	1.025	0.639	0.047
Butyl formate	$C_5H_{10}O_2$	2.658	0.862	1.397	1.540	1.019
Ethyl propanoate	$C_5H_{10}O_2$	2.266	0.223	0.458	0.339	0.131
Propyl acetate	$C_5H_{10}O_2$	0.879	1.190	1.174	0.146	0.049
Sec butyl formate	$C_5H_{10}O_2$	2.770	2.671	3.822	3.327	1.072
Iso Pentane	C_5H_{12}	1.145	0.003	0.232	0.117	0.002
Neopentane	C_5H_{12}	8.185	0.930	5.876	7.318	0.912
Pentane	C_5H_{12}	1.360	0.005	0.311	0.266	0.004
1-Pentanol	$C_5H_{12}O$	5.089	0.118	5.771	5.084	0.007
2-Pentanol	$C_5H_{12}O$	7.656	0.388	8.597	8.328	0.237
Ethyl propyl ether	$C_5H_{12}O$	6.802	0.118	5.385	4.442	0.046
Methyl butyl ether	$C_5H_{12}O$	1.278	0.112	0.521	1.283	0.100
Diethoxymethane	$C_5H_{12}O_2$	8.745	0.136	6.924	6.290	0.210
Propyl cellosive	$C_5H_{12}O_2$	4.844	0.407	3.302	2.494	0.433
Isoperene	C_5H_8	8.140	0.035	11.072	3.366	0.020
Spiropentane	C_5H_8	4.905	0.010	3.778	16.864	0.720
2,3-Dimethyl-1,3-butadien	C_6H_{10}	6.359	0.119	10.371	4.570	0.088
3-Hexyne	C_6H_{10}	10.931	2.106	15.538	7.447	0.826

Table 2. Continued

1-Hexene	C_6H_{12}	1.278	0.008	0.394	1.102	0.007
2,3-Dimethyl-2-butene	C_6H_{12}	4.926	0.005	6.883	2.592	0.003
3,3-Dimethyl-1-butene	C_6H_{12}	3.052	0.021	1.165	0.676	0.019
Cyclohexane-1	C_6H_{12}	0.211	0.014	2.391	0.418	0.008
Cyclohexane-2	C_6H_{12}	0.615	0.112	4.228	0.455	0.040
Cyclohexanol	$C_6H_{12}O$	16.604	1.157	18.605	9.986	0.692
Butyl acetate	$C_6H_{12}O_2$	2.282	0.078	0.659	1.761	0.094
2,2-Dimethyl butane	C_6H_{14}	1.594	0.007	0.363	0.415	0.007
2,3-Dimethyl butane	C_6H_{14}	1.780	0.007	0.318	0.671	0.006
2-Methyl pentane	C_6H_{14}	1.210	0.016	0.245	0.768	0.010
2-Methyl pentane	C_6H_{14}	2.123	0.011	0.547	11.596	0.009
Hexane	C_6H_{14}	2.107	0.010	0.487	0.771	0.008
1-Hexanol	$C_6H_{14}O$	21.798	0.822	24.623	26.730	0.537
2-Hexanol	$C_6H_{14}O$	8.487	4.963	9.970	10.758	1.523
2-Methyl-1-pentanol	$C_6H_{14}O$	18.590	5.921	21.837	22.302	1.552
2-Methyl-4-pentanol	$C_6H_{14}O$	4.043	2.196	4.578	4.382	2.839
3-Hexanol	$C_6H_{14}O$	4.287	5.318	5.515	5.946	0.836
DiIsopropyl ether	$C_6H_{14}O$	1.711	0.058	0.442	0.712	0.047
Dipropyle ether	$C_6H_{14}O$	3.652	0.069	2.135	2.813	0.068
Ethyl butyl ether	$C_6H_{14}O$	2.357	0.052	1.134	2.178	0.049
Benzene	C_6H_6	0.501	0.009	2.641	0.680	0.009
Phenol	C_6H_6O	2.039	2.207	4.753	0.709	0.025
Resorcinol	$C_6H_6O_2$	4.245	1.584	3.047	3.571	1.800
Pyrogallol	$C_6H_6O_3$	9.636	5.323	9.766	9.830	1.972
1,1-Dimethylcyclopentane	C_7H_{14}	5.227	0.032	3.008	2.327	0.023
1-Heptene	C_7H_{14}	3.778	0.048	1.929	2.224	0.043
Cis-1,2-dimethylcyclopentane	C_7H_{14}	3.500	0.511	1.138	1.695	0.673
Cis-1,3-dimethylcyclopentane	C_7H_{14}	2.015	0.010	1.001	1.500	0.008
Cycloheptane	C_7H_{14}	1.239	0.008	0.272	0.302	0.007
Ethylcyclopentane	C_7H_{14}	1.848	0.023	0.517	0.873	0.021
Methylcyclohexane	C_7H_{14}	1.370	0.456	1.151	0.607	0.012
Trans-1,2-dimethylcyclopentane	C_7H_{14}	3.772	0.013	1.648	1.551	0.014
Trans-1,3-dimethylcyclopentane	C_7H_{14}	7.782	0.027	5.401	5.829	0.023
2,4-Dimethyl-3-pentanone	$C_7H_{14}O$	5.224	0.174	3.220	4.223	0.112
Butyl propanoate	$C_7H_{14}O_2$	4.003	0.964	6.144	4.720	0.735
Heptanoic acid	$C_7H_{14}O_2$	7.379	1.249	8.237	11.034	1.091
2,2-Dimethylpentane	C_7H_{16}	1.758	0.043	0.114	0.773	0.055
2,3-Dimethylpentane	C_7H_{16}	2.010	0.085	0.179	1.249	0.162

Table 2. Continued

2,4-Dimethylpentane	C_7H_{16}	1.905	0.023	0.620	1.170	0.007
2-Methylhexane	C_7H_{16}	1.489	0.023	0.673	1.289	0.014
3-Ethylpentane	C_7H_{16}	1.618	0.022	0.829	1.003	0.019
3-Methylhexane	C_7H_{16}	3.597	2.074	3.047	3.519	1.245
Heptane	C_7H_{16}	1.938	0.024	0.126	1.086	0.027
Toluene	C_7H_8	2.689	0.139	0.275	0.926	0.138

Table 3. Statistical Parameters of the Proposed Equation Against Other Methods

	AARD%	RMSD
Antoine	0.625	2.832
Ambros-walton	3.840	7.241
Riedel	3.624	7.002
Lee-kesler	4.383	6.468
This study	0.333	0.872

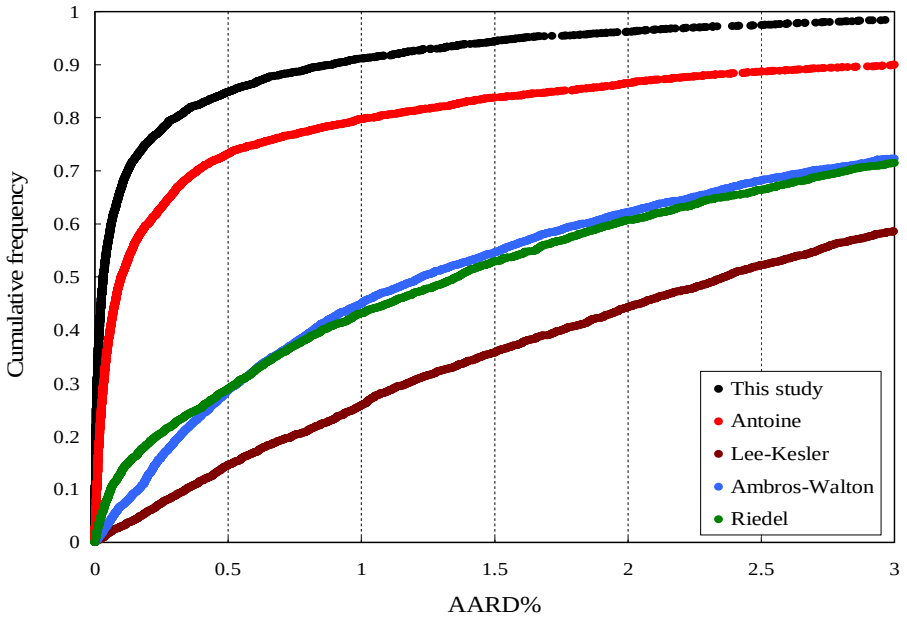

Fig. 2. Cumulative frequency of literature and new method as a function of AARD%.

accurate than all literature methods for all of the pure substances considered in this work.

Table 3 presents the statistical parameters including average absolute relative deviation (AARD%) and root mean square deviation (RMSD) of the literature correlations and new developed equation.

Figure 2 shows the cumulative frequency of the proposed model and different literature methods versus average absolute relative deviations. Figure 2 also shows the accuracy of all considered methods in prediction of vapor pressure of 130 substances. As shown in Fig. 2, developed equation is more accurate than four commonly used models in vapor pressure prediction.

The new method has successfully predicted 85% of all experimental data with AARD% less than 0.5, and 96.3% of the data with AARD% less than 2. Only 1% of the vapor pressure data were predicted with AARD% of more than 3 by the new method. Antoine equation, that is the second accurate method, predicted 73% of the data with AARD (%) less than 0.5, and 86% of the data with AARD (%) less than 1. Hence the superiority of this new method over the literature correlations has been verified for all data existing in data bank.

CONCLUSIONS

In this study, various vapor pressure correlations in literature and a new developed model are evaluated and compared with each other. It is found that undesirable predicting deviations are obtained using the Antoine equation, Lee-Kesler method, Ambrose-Walton method, and Riedel Method over a wide ranges of temperature. The Antoine method generally gives good prediction accuracy relative to the other literature models. Four literature non-linear correlations were used to estimate the vapor pressure of C-H-O pure substances, being a function of reduced temperature and critical pressure. To validate the proposed method, the vapor pressures of 130 C-H-O pure substances with more than 2019 experimental data points were examined and an overall average absolute relative deviation of 0.333% was achieved.

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