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Review of Vapor Pressure Correlation

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Abstract

This work reviews the experimental data and correlations vapor pressure for eight organic compounds, including (ethane,90.36-300K; pentane,309.2-469.6K; ethene(ethylene),103.99-276K; ethyne (acetylene),192.2-308.7K; 1,1-difluoroethane(R152a), 154.56-378K; benzene,278.7-550K; toluene,383.78-594K and 1,3-dimethylbenzene (m- Xylene),412-617K) are reported, and the four predictive correlations including Antoine, Wagner, Lee–Kesler'sand Clausius-Clapeyron, this various correlations are evaluated and compared with experimental data. The results indicate that Lee–Kesler'swithAAPD of 1.78%, WagnerwithAAPD of 2.37%, Antoine withAAPD of 2.73% and Clausius-ClapeyronwithAAPD of 8.63% was achieved. It is shown that the Lee–Kesler's equation is more accurate than three commonly used models in vapor pressure prediction.

Keywords:

Thermodynamics;
Organic Compounds;
Saturated Temperature;
Vapor Pressure Correlation;

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1. Introduction

Thermodynamic properties of chemical compounds such as vapor pressure are very important in design of different industries for instant petrochemical and chemical processes.

They are several methods are used for the determination of vapor pressure of organic and inorganic compounds. The most important among them are Antoine equation method [1], Wagner equation method [1], Lee–Kesler's Method [2],Clausius-Clapeyron equation method [1]and experimental methods. It should be noted that the comparison of correlations is very important to demonstrate and to give deeper knowledge which one is more accurate.

2. Vapor Pressure Correlations

Generalized correlation of vapor pressure they have exist a number of correlations of vapor pressure of pure fluids. These include:

2.1 Wagner equation method

Wagner (1973, 1977) used an elaborate statistical method to develop an equation forrepresenting the vapor pressure behavior[1], Wagner correlation (eqn. 1) has a wide range of validity down to T_r= 0.5 [41].

$$\ln P_r^s = (a + b\tau^{1.5} + c\tau^{2.5} + d\tau^5)(1-\tau)^{-1} \quad (1)$$

where

$$\tau = 1 - T_r, T_r = \frac{T}{T_c}$$

Wagner constants (a, b, c, d, …)are depend on fluid specific. Hence a large data bank is needed for each fluid coefficient.

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Table1. Wagner correlation constants [3]

Compound	Wagner correlation constants			
	a	b	c	d
Ethane	-6.475	1.411	-1.144	-1.859
Pentane	-7.307	1.758	-2.163	-2.913
Ethene(Ethylene)	-6.321	1.168	-1.559	-1.836
Ethyne(Acetylene)	-6.901	1.269	-2.091	-2.756
1,1-Difluoroethane (R152a)	-7.433	1.756	-2.170	-2.775
Benzene	-7.014	1.553	-1.848	-3.713
Toluene	-7.316	1.594	-1.932	-3.722
1,3-dimethylbenzene (m- Xylene)	-7.677	1.802	-2.477	-3.661

2.2 Antoine equation method

Antoine, C.; Compt. rend., (1988). Proposed a simple modification and it has been widely used over limited temperature ranges.

$$\ln P^s = A - \frac{B}{C+T} \quad (2)$$

Where T is in Kelvin. When C = 0. Although Antoine correlation equation (2) is widely used, Simple rules have been proposed (Fishtine,1963; Thompson, 1959) to relate C to the normal boiling point for certain classes of materials, but these rules are not reliable.

and the only reliable way to obtain values of the constants A, B, and C is to regress experimental data and it depend on fluid specific.

Table2: Antoine correlation coefficients [5]

Compound	Antoine correlation coefficients			
	A	B	C	Temperature range(K) T_{min}, T_{max}
Ethane	6.953	699.106	260.264	90.35, 305.42
Pentane	7.009	1134.15	238.678	143.42, 469.65
Ethene(Ethylene)	6.966	649.806	262.73	104.01, 282.36
Ethyne(Acetylene)	7.315	790.209	262.859	192.4, 308.32
1,1-Difluoroethane (R152a)	7.120	928.549	244.854	156.15, 386.6
Benzene	7.064	1296.93	229.916	278.68, 562.16
Toluene	7.136	1457.29	231.827	178.18, 591.79
1,3-dimethylbenzene (m- Xylene)	7.181	1573.02	226.671	225.3, 617.05

2.3 Clausius-Clapeyron equation method

Poling, E; Prausnitz, M; O'connel, P,(2001).reported, that the Clausius-Clapeyron equation (eqn. 3) of vapor pressure is.

$$\ln P_{vpr} = h(1 - \frac{1}{T_r}) \quad (3)$$

where:

$$h = T_{br}\frac{\ln(P_c/1.01325)}{1-T_{br}} \quad (4)$$

Surprisingly, it is a fairly good relation for approximating vapor pressure over small temperature intervals.

2.3 Lee–Kesler's Methodmethod

The vapor pressure can obtain by Lee–Kesler's method [2] is one of the successful methods to predict the vapor pressure using the three-parameter formulations [4] equation (5).

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

Where:

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.2886\ln T_r + 0.16935.T_r^{\,6}$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.472\ln T_r + 0.4358.T_r^{\,6}$$

Table3. Physical constants of organic compounds [7]

No	Compound	Formula	M	T_b(K)	T_c(K)	P_c(bar)	T_{br}	ω
1	Ethane	C2H6	30.070	184.55	305.33	48.718	0.60	0.099
2	n-Pentane	C5H12	72.151	309.22	469.6	33.69	0.66	0.251
3	Ethene(Ethylene)	C2H4	28.054	169.42	282.34	50.401	0.60	0.087
4	Ethyne(Acetylene)	C2H2	26.038	188.40	308.32	62.4	0.61	0.188
5	1,1-difluoroethane (R152a)	C2H4F2	66.052	249.10	386.41	45.17	0.64	0.276
6	Benzene	C6H6	78.114	353.24	562.05	48.95	0.63	0.209
7	Toluene	C6H5CH3	92.141	383.79	591.8	41.08	0.65	0.262
8	1,3-dimethylbenzene (m- Xylene)	C8H10	106.17	412.34	617	35.43	0.67	0.325

3. Results and Discussion

We carried out calculations for eight different pure organic compounds, such as ethane, pentane, ethyne (ethylene), ethene (acetylene),
1,1-difluoroethane(R152a), benzene, toluene and 1,3-dimethylbenzene (m- Xylene).The values of the Antoine, Wagner, Lee–Kesler's and Clausius-Clapeyroncorrelation coefficients, experimental vapor pressure data, temperature, critical pressure, critical temperature, boiling point, reduced boiling point and acentric factor, (used for calculation of literature models) were taken from data bank to estimate the values of vapor pressure of fourcorrelations.

Table4. Vapor pressure of organic compounds

No	Temperature (K) T_{min}, T_{max}	Experimental vapor pressure (mmHg) Source: Ref.[17]	Antoine vapor pressure (mmHg)	Wagner vapor pressure (mmHg)	Lee–Kesler's vapor pressure (mmHg)	Clausius-Clapeyron vapor pressure (mmHg)
Ethane						
1	90.360	0.007	0.008497	0.008425	0.009005	0.028092
2	120	2.625	2.668411	2.659924	2.536475	3.922753
3	150	72.456	71.49559	72.55021	69.42429	79.69588
4	184.56	759.963	759.8219	760.3266	749.4885	760.4033
5	200	1629.734	1647.187	1630.387	1622.959	1619.126
6	220	3691.579	3780.378	3692.616	3701.733	3680.999
7	240	7253.246	7495.209	7254.676	7283.461	7297.988
8	260	12844.81	13302	12842.47	12872.38	13023.02
9	280	21058.73	21664.21	21051.45	21065.46	21393.93
10	300	32683.19	32965.36	32677.09	32702.88	32894.67
n-Pentane						
1	309.2	759.813	759.862	761.4482	756.2023	759.4958
2	335	1702.64	1718.47	1699.976	1705.522	1673.844
3	350	2557.71	2597.46	2551.483	2567.966	2511.796
4	365	3690.303	3781.568	3691.928	3721.154	3645.573
5	380	5160.424	5328.833	5177.569	5218.898	5137.776
6	395	7013.077	7297.888	7068.954	7119.092	7054.517
7	410	9368.27	9746.583	9432.189	9486.15	9464.21
8	425	12256.01	12730.78	12341.68	12395.01	12436.36
9	440	15773.8	16303.31	15885.8	15937.05	16040.4
10	469.6	25269.58	25265.37	25269.58	25269.58	25269.58
Ethene(Ethylene)						
1	103.99	0.915	1.050515	0.575552	0.996031	1.627465
2	125	18.962	19.71518	14.04228	19.08561	23.61738
3	150	205.367	204.4383	172.3084	202.753	214.5672
4	169.4	758.312	756.2331	681.383	754.4	759.124

5	185	1750.944	1753.435	1628.544	1744.845	1730.187
6	205	4171.693	4231.25	4015.261	4173.878	4141.236
7	225	8457.696	8664.247	8318.834	8463.926	8487.553
8	245	15282.51	15700.64	15214.71	15269.26	15472.23
9	260	22528.1	23035.73	22522.92	22499.17	22845.63
10	276	32800.95	36496.99	32822.41	32804.32	33041.46
Ethyne(Acetylene)						
1	192.2	960.079	935.4494	836.4182	952.2076	937.0796
2	200	1417.617	1411.321	1292.966	1446.091	1404.948
3	210	2280.188	2281.381	2139.649	2346.146	2259.641
4	230	5167.925	5228.578	5046.03	5355.392	5163.683
5	240	7395.608	7498.187	7296.751	7638.969	7412.882
6	250	10275.85	10434.35	10214.45	10565.11	10338.38
7	270	18376.51	18721.01	18483.5	18758	18675.82
8	280	23926.97	24274.05	24069.22	24267.29	24318.38
9	290	30602.52	30895.05	30803.13	30922.03	31094.42
10	308.7	46803.85	46443.65	46331.32	47193.41	47178.3
1,1-Difluoroethane (R152a)						
1	154.56	0.525	0.583407	0.480703	0.402998	1.101811
2	190	20.852	23.86294	20.81867	18.58313	27.36845
3	220	171.164	188.947	171.2681	161.6323	184.9053
4	249.13	759.813	822.7398	760.1536	746.0479	760.9786
5	270	1766.47	1898.112	1766.159	1763.078	1738.015
6	290	3491.012	3731.74	3489.095	3512.428	3430.364
7	310	6270.216	6665.201	6264.843	6322.156	6201.91
8	330	10453.61	11023.46	10442.87	10524.8	10436.06
9	350	16444.35	17125.93	16429.05	16514.44	16546.96
10	378	28884.13	29157.97	28877.32	28941.28	29065.93
Benzene						
1	278.7	35.928	35.98082	36.01397	36.69778	46.6085
2	300	103.584	103.0341	103.8288	104.0527	119.2276
3	325	291.099	289.1599	291.5822	290.3568	306.8601
4	353.3	761.313	760.756	762.528	760.0534	761.3483
5	400	2642.467	2683.861	2645.778	2651.192	2574.591
6	450	7287.599	7509.425	7292.463	7314.884	7169.443
7	475	11115.16	11487.36	11119.41	11139.64	11034.69
8	500	16249.34	16773.55	16252.98	16260.94	16266.99
9	525	22958.64	23548.7	22968.42	22969.49	23110.11
10	550	31618.85	31972.12	31638.69	31659.75	31800.5
Toluene						
1	383.78	759.813	759.6341	760.1523	756.257	759.7915
2	400	1185.097	1183.153	1178.811	1179.731	1164.661
3	425	2137.676	2176.602	2151.419	2166.794	2110.516
4	450	3652.8	3716.445	3644.497	3681.303	3580.06
5	475	5820.479	5966.066	5812.884	5871.762	5744.257
6	500	9225.759	9095.791	8827.956	8900.22	8791.097
7	525	13651.12	13275.76	12881.62	12952.03	12919.67
8	550	19276.59	18669.68	18198.59	18255.86	18334.07
9	575	25877.13	25429.68	25071.84	25117.06	25237.62
10	594	30377.5	31565.72	31202.23	31633.57	31602.04
1,3-dimethylbenzene (m- Xylene)						
1	412	759.813	754.2216	754.7796	752.3366	753.309
2	430	1215.1	1200.819	1196.743	1200.713	1180.162
3	455	2107.673	2140.306	2118.081	2137.394	2075.584
4	480	3540.291	3568.825	3506.618	3546.633	3441.893
5	505	5557.957	5628.09	5497.181	5557.472	5428.829
6	530	8408.191	8467.185	8240.603	8313.452	8202.464
7	555	12008.49	12237.04	11909.05	11982.63	11940.84

8	580	16981.4	17085.39	16710.57	16776.6	16829.3
9	605	22891.88	23152.47	22932.09	22981.5	23055.81
10	617	26574.69	26536.03	26574.69	26574.69	26574.69

Table5. Percent Deviation of Antoine, Wagner, Lee-Kesler's and Clausius correlations

No	Temperature (K) T_{min}, T_{max}	Antoine vapor pressure (mmHg) $\|PD\|$	Wagner vapor pressure (mmHg) $\|PD\|$	Lee–Kesler's vapor pressure (mmHg) $\|PD\|$	Clausius-Clapeyron vapor pressure (mmHg) $\|PD\|$
Ethane					
1	90.360	4.90	4.01	11.17	246.82
2	120	1.65	1.33	3.37	49.44
3	150	1.33	0.13	4.18	9.99
4	184.56	0.02	0.05	1.38	0.06
5	200	1.07	0.04	0.42	0.65
6	220	2.41	0.03	0.28	0.29
7	240	3.34	0.02	0.42	0.62
8	260	3.56	0.02	0.21	1.39
9	280	2.88	0.03	0.03	1.59
10	300	0.86	0.02	0.06	0.65
n-Pentane					
1	309.2	0.01	0.22	0.48	0.04
2	335	0.93	0.16	0.17	1.69
3	350	1.55	0.24	0.40	1.80
4	365	2.47	0.04	0.84	1.21
5	380	3.26	0.33	1.13	0.44
6	395	4.06	0.80	1.51	0.59
7	410	4.04	0.68	1.26	1.02
8	425	3.87	0.70	1.13	1.47
9	440	3.36	0.71	1.03	1.69
10	469.6	0.017	0	0	0
Ethene(Ethylene)					
1	103.99	14.81	37.10	8.86	77.87
2	125	3.97	25.95	0.65	24.55
3	150	0.45	16.10	1.27	4.48
4	169.4	0.27	10.14	0.52	0.11
5	185	0.14	6.99	0.35	1.19
6	205	1.43	3.75	0.05	0.73
7	225	2.44	1.64	0.07	0.35
8	245	2.74	0.44	0.09	1.24
9	260	2.25	0.02	0.13	1.41
10	276	11.27	0.07	0.01	0.73
Ethyne(Acetylene)					
1	192.2	2.57	12.88	0.82	2.40
2	200	0.44	8.79	2.01	0.89
3	210	0.05	6.16	2.89	0.90
4	230	1.17	2.36	3.63	0.08
5	240	1.39	1.34	3.29	0.23
6	250	1.54	0.60	2.81	0.61
7	270	1.87	0.58	2.08	1.63
8	280	1.45	0.59	1.42	1.64

9	290	0.96	0.66	1.04	1.61
10	308.7	0.77	1.01	0.83	0.80
1,1-Difluoroethane (R152a)					
1	154.56	11.12	8.44	23.24	109.87
2	190	14.44	0.16	10.88	31.25
3	220	10.39	0.06	5.57	8.03
4	249.13	8.28	0.04	1.81	0.15
5	270	7.45	0.02	0.19	1.61
6	290	6.90	0.05	0.61	1.74
7	310	6.30	0.09	0.83	1.09
8	330	5.45	0.10	0.68	0.17
9	350	4.14	0.09	0.43	0.62
10	378	0.95	0.02	0.20	0.63
Benzene					
1	278.7	0.15	0.24	2.14	29.73
2	300	0.53	0.24	0.45	15.10
3	325	0.67	0.17	0.25	5.41
4	353.3	0.07	0.16	0.17	0.00
5	400	1.57	0.13	0.33	2.57
6	450	3.04	0.07	0.37	1.62
7	475	3.35	0.04	0.22	0.72
8	500	3.23	0.02	0.07	0.11
9	525	2.57	0.04	0.05	0.66
10	550	1.11	0.06	0.13	0.57
Toluene					
1	383.78	0.02	0.04	0.47	0.00
2	400	0.16	0.53	0.45	1.72
3	425	1.82	0.64	1.36	1.27
4	450	1.74	0.23	0.78	1.99
5	475	2.50	0.13	0.88	1.31
6	500	1.41	4.31	3.53	4.71
7	525	2.75	5.64	5.12	5.36
8	550	3.15	5.59	5.30	4.89
9	575	1.73	3.11	2.94	2.47
10	594	3.91	2.71	4.13	4.03
1,3-dimethylbenzene (m- Xylene)					
1	412	0.74	0.66	0.98	0.86
2	430	1.18	1.51	1.18	2.88
3	455	1.55	0.49	1.41	1.52
4	480	0.81	0.95	0.18	2.78
5	505	1.26	1.09	0.01	2.32
6	530	0.70	1.99	1.13	2.45
7	555	1.90	0.83	0.22	0.56
8	580	0.61	1.59	1.21	0.90
9	605	1.14	0.18	0.39	0.72
10	617	0.15	0	0	0

Table6. Comparison of Vapor Pressure correlations

Compound	No. of data points	Antoine	Wagner	Lee–Kesler's	Clausius-Clapeyron
Ethane	10	2.20	0.57	2.15	31.15
Pentane	10	2.36	0.39	0.80	0.10
Ethene(Ethylene)	10	3.98	10.22	1.2	11.27
Ethyne(Acetylene)	10	1.22	3.50	2.08	1.08
1,1-Difluoroethane (R152a)	10	7.54	0.91	4.44	15.52
Benzene	10	1.63	0.12	0.42	5.65
Toluene	10	1.92	2.29	2.50	2.78
1,3-dimethylbenzene (m- Xylene)	10	1.00	0.93	0.67	1.50
AAPD		**2.73**	**2.37**	**1.78**	**8.63**

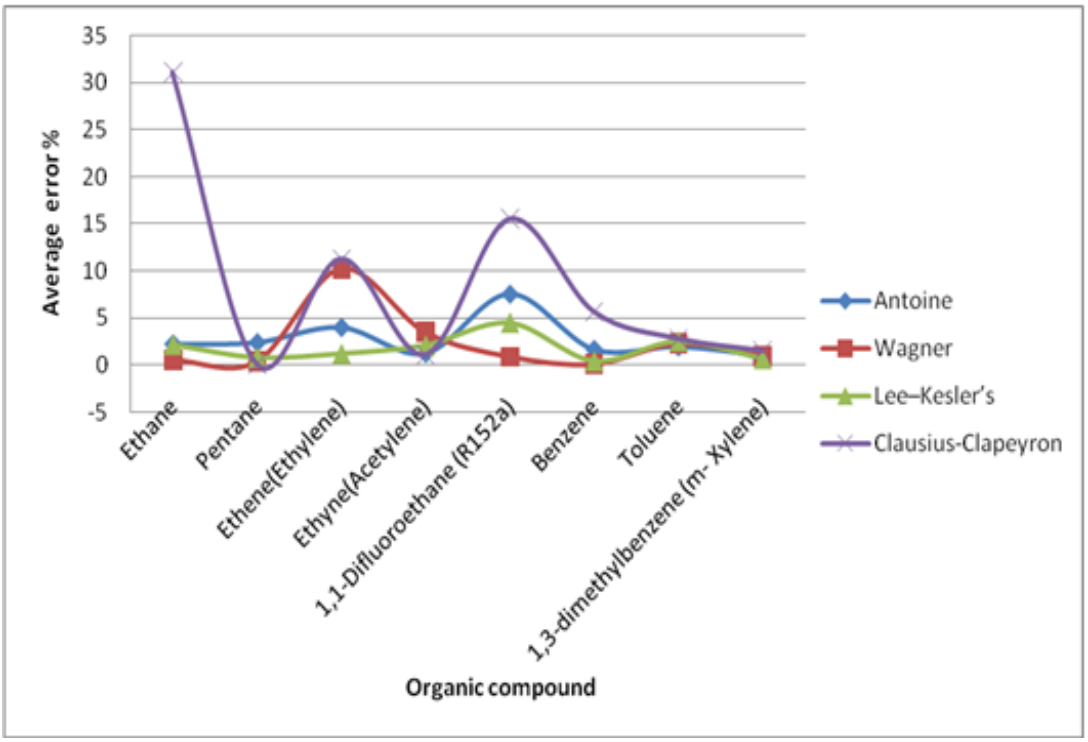

Figure1*: Average error*

Table 1 shows the Wagner equation constants of the each eight organic compounds using the given entire-curve Wagner constants.
Table 2 shows the Antoine correlation coefficients with maximum and minimum temperature ranges of organic compound under this study.
Table 3 shows physical constant of organic compounds such as molecular weight, boiling point, critical temperatures, critical pressures, reduced boiling point and acentric factor.
Table 4 shows the results of vapor of the experimental of literature and four correlations indicate the equations 1, 2, 3 and 5 can predict vapor pressure of organic compounds.
Table 6 compares experimental vapor pressures of organic compounds versus corresponded values of Antoine, Wagner, Lee–Kesler'sand Clausius-Clapeyroncorrelations are presented in Figure 1.

In Table 6, average error of the calculated vapor pressure of four correlations for all 8 substances with 80 data points are presented in this work, the results have Lee–Kesler'swith AAPD of 1.78%, Wagnerwith AAPD of 2.37%, Antoinewith AAPD of 2.73% and Clausius-Clapeyronwith AAPD of 8.63% respectively.
Table 6 also shows Lee–Kesler's equation is more accurate than three commonly used models in vapor pressure prediction.

4. Conclusion

For the review of vapor pressure of ethane, pentane, ethene(ethylene), ethyne(acetylene), 1,1-difluoroethane(R152a), benzene, toluene and 1,3-dimethylbenzene (m- Xylene), four predictive models including Antoine, Wagner, Lee–Kesler'sand Clausius-Clapeyron, this various correlations are evaluated and compared with experimental data. It is found that the vapor pressure predicting deviations are obtained using the Antoine equation, Wagner, Lee–Kesler'sand Clausius-Clapeyronmethod over wide ranges of temperature.
Correlations used to estimate the vapor pressure of each organic compound. To evaluate the four equations, the vapor pressures of 8 organic compounds with 80 experimental data points were examined and Lee–Kesler'swithAAPD of 1.78%, WagnerwithAAPD of 2.37%, Antoine withAAPD of 2.73% and Clausius-ClapeyronwithAAPD of 8.63% was achieved. Also, in this work Lee–Kesler's equation is more accurate than three commonly used models in vaporpressure prediction.

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