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Statistical investigations for predicting the boiling temperature of some liquid solvents through the viscosity-temperature dependence

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INTRODUCTION

Knowledge and estimation of transport properties of fluids are necessary for mass flow and heat transfer. Viscosity is one of the main properties which are sensitive to temperature and pressure variation. In the present work, based on the use of statistical techniques for regression analysis and correlation tests, we propose an original equation modeling the relationship between the two parameters of viscosity Arrhenius-type equation (Eq. 1). Empirical validation using 76 data set of fluids provided from the literature and studied at different temperature ranges gives excellent statistical results. More, causal correlation between these parameters and the normal boiling temperature (Tb) of the corresponding fluids leads us to propose two predictive empirical equations one with the activation energy (Eq. 3) and one with the logarithm of pre-exponential factor (Eq. 4). We conclude that the boiling temperature is in causal correlation with the two Arrhenius parameters, (lnAs) and (Ea). Note that Alkhaldi equation is tested to some heavy oils with reliable agreement for which we can conclude that it can be useful for petroleum chemistry and industrial Chemistry.

Key words Pure liquid · Arrhenius activation energy · Boiling temperature · Arrhenius temperature. Solvents . Correlation

Arrhenius-Type Equation

$$\eta = As \cdot exp\left(\frac{Ea}{RT}\right) \quad (1)$$

$$ln\eta = lnAs + \frac{Ea}{RT} \quad (2)$$

$$Arrhenius\ Temperature: T_A = -\frac{1000.Ea}{R.lnAs}$$

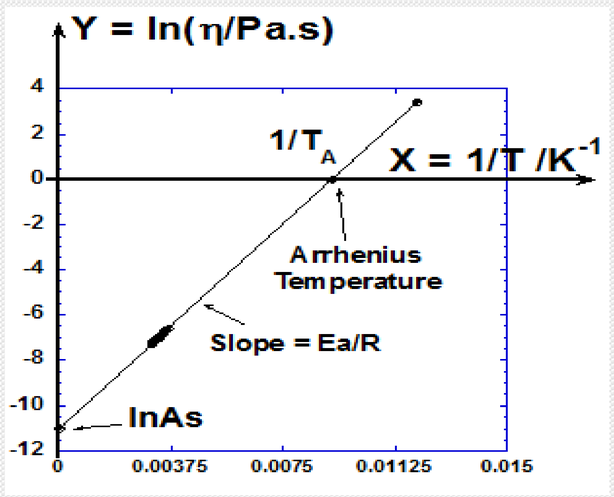


Figure 1 : This plot shows how to determine graphically (**Ea/R**), (**lnAs**) and (T_A). We have proceeded by **extrapolation** to reach these two parameters…

Mutual correlations between Arrhenius parameters

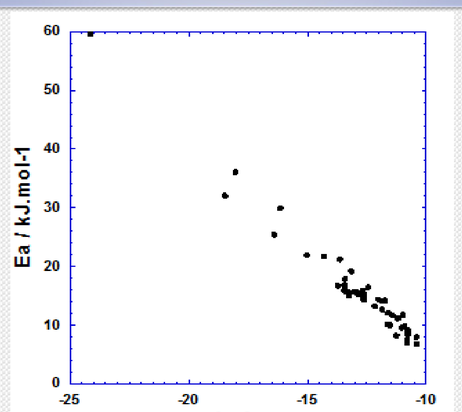


Figure 2 : Correlation between the Arrhenius activation energy Ea / (kJ•mol^{-1}), and the logarithm of the entropic factor of Arrhenius – R•ln(As/Pa•s) / (J•K^{-1}•mol^{-1}) for some pure solvents.

Correlation between Arrhenius parameters and boiling temperature

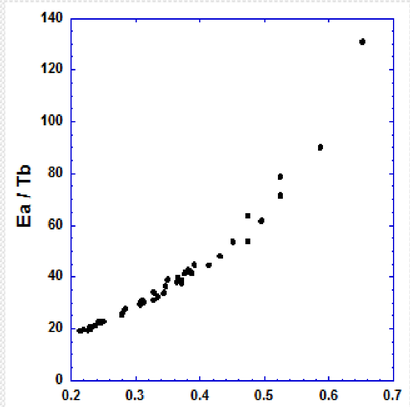


Figure 3 : Correlation between the ratios and Arrhenius activation energy-boiling point (Ea/T_b) and the Arrhenius temperature-boiling point (T_A /T_b) for some pure solvents.

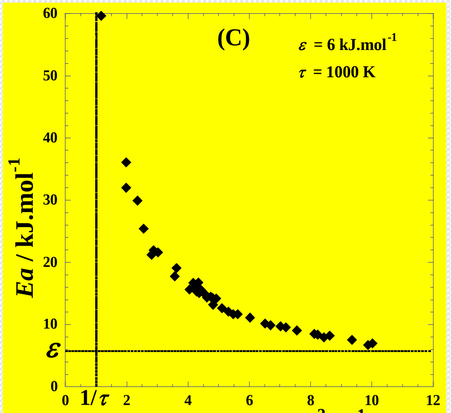


Figure 4. Correlations between *Ea* and transformed variables as a function of ($1/T_A$ and $1/T_b$) of some pure liquids .

Prediction of boiling point via viscosity Arrhenius parameters

$$T_b(E_a) = -\frac{E_a}{68 - 4.05 \times Ea^{0.34}} \quad (3)$$

$$(4)\quad T_b(lnA_s) = \frac{(-lnA_s)^{2.933}}{8.2 + lnA_s}$$

$$E_a = \frac{R.\omega}{\left(\frac{1}{T_A} - \frac{1}{T_b}\right) - \frac{1}{\tau}} + \varepsilon_0$$

New Equation

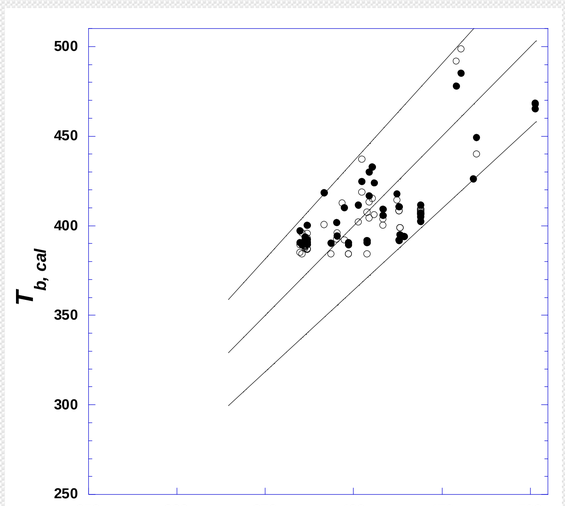


Figure 5 : Correlation between the experimental boiling temperature $T_{b,exp}$ / K and the calculated boiling temperature ($T_{b,cal}$) / K for some pure liquids studied at previous work [1]; (●): from Eq. 3 and (○): from Eq. 4). (—): around the first bisector (*Y* = +*X* and *Y* = (1±9%)×*X*) in the present axis system.

Scholars' List

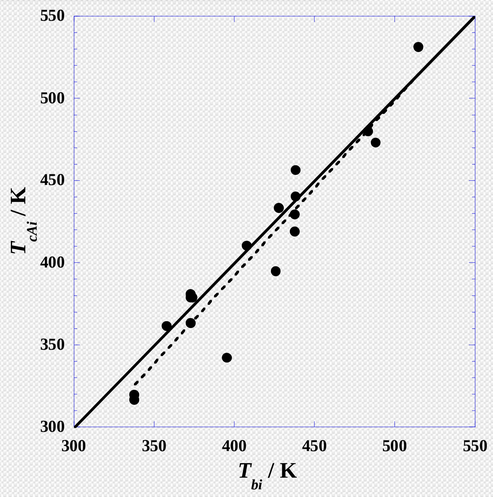
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$$Activations\ Temperature: T^* = \frac{Ea}{1000.R}$$

Parameters	Arithmetic Mean	Quadratic Mean	Standard Deviation	Standard Error	Confidence Interval	Coefficient of Variation
Ea	17.407	20.681	11.242	1.2895	14.828 – 19.986	65%
lnAs	-13.299	13.634	3.0237	0.34684	-13.993 – -12.605	23%
T_A	146.19	155.66	53.829	6.1746	133.89 – 158.49	37%
T_m	229.16	234.50	50.068	5.7432	217.72 – 240.60	22%
T_b	403.23	406.24	49.718	5.7031	391.87 – 414.58	12%
*T**	2093.55	2487.4	1352.1	155.09	1784.59 – 2402.52	65%

Table 2. Descriptive statistics on different parameters.



Pure Component	lnAs	Ea	T_A	T*	T_b	T_m
	-	/ kJ.mol^{-1}	/ K	/ K	/ K	/ K
Water	-13.414	15.835	141.98	1904.5	373.15	273.15
Benzene	-11.812	10.940	111.39	1315.8	353.15	278.65
Chlorobenzene	-10.695	8.7094	97.939	1047.5	405.15	228.15
ethylbenzene	-11.027	9.1110	99.375	1095.8	409.15	178.15
o-xylene	-11.145	9.8360	106.14	1183.0	417.15	248.65
n-heptane	-11.302	8.6196	91.723	1036.7	371.15	182.55
n-pentane	-10.886	6.0998	67.393	733.64	309.25	143.45
Toluene	-11.135	9.0229	97.461	1085.2	383.75	180.15
m-xylene	-10.975	8.7485	95.872	1052.2	412.25	225.35
Carbone tetrachloride	-11.152	10.329	111.39	1242.3	349.87	250.23
Ethyl acetate	-11.728	9.9183	101.72	1192.9	350.15	189.55
Diethyl ether	-11.446	7.5203	79.021	904.48	307.75	156.85
Acetic acid	-11.308	11.213	119.26	1348.6	391.15	289.75
Acetone	-11.097	7.4406	80.643	894.9	329.20	178.45
Butyl Alcohol	-13.689	19.114	167.94	2298.9	390.85	183.35
Aniline	-13.564	19.997	177.32	2405.1	457.28	266.85
n-octanol	-14.945	24.955	200.83	3001.4	468.15	257.15
Propylene Glycol	-22.128	47.765	259.62	5744.8	461.35	214.15
Butane-1,4-diol	-16.210	33.359	247.51	4012.2	503.15	293.15
Butane-1,2-diol	-20.681	43.910	255.36	5281.1	465.15	159.15
1,4-Butanediol	-16.438	33.904	248.07	4077.7	503.15	293.15
1,4-Butanediol	-16.485	34.033	248.31	4093.3	503.15	293.15
1,2-Butanediol	-21.510	45.933	256.84	5524.5	465.15	159.15
1,2-Butanediol	-21.857	46.763	257.32	5624.3	465.15	159.15
Propylene Glycol	-18.266	37.551	247.25	4516.3	461.35	214.15
N,N-dimethylformamide	-10.780	9.0530	101.00	1088.8	425.00	212.15
Formamide	-12.442	16.410	158.63	1973.7	483.15	275.65
N,N-dimethylacetamide	-10.914	9.7590	107.54	1173.7	438.55	253.15
2-Methoxyethanol	-12.602	15.185	144.93	1826.3	397.65	188.15
Water	-13.284	15.510	140.42	1865.4	373.15	273.15
N,N-dimethylacetamide	-10.896	9.4260	104.05	1133.7	438.55	253.15
2-Ethoxyethanol	-12.682	15.803	149.87	1900.7	408.15	183.15
N,N-dimethylacetamide	-10.934	9.7973	107.77	1178.3	438.55	253.15
1,4-dioxane	-11.853	12.660	128.47	1522.6	374.15	284.15
Water	-13.443	15.920	142.43	1914.7	373.15	273.15
Isobutyric acid	-11.200	11.126	119.48	1338.1	426.65	226.15
Water	-13.383	15.749	141.54	1894.2	373.15	273.15
Ethanol	-12.166	13.204	130.50	1588.1	351.15	159.15
Water	-13.232	15.433	140.28	1856.2	373.15	273.15
Methanol	-11.528	9.9340	103.64	1194.8	337.75	175.55
Water	-13.334	15.640	141.07	1881.1	373.15	273.15
p-xylene	-10.761	8.3920	93.800	1009.3	411.15	285.65
Dimethylsulfoxide	-11.872	14.058	142.42	1690.8	462.15	290.65
o-xylene	-11.044	9.5730	104.26	1151.4	417.15	248.65
Dimethylsulfoxide	-12.002	14.333	143.63	1723.9	462.15	290.65
Ethylene glycol	-16.146	29.941	223.03	3601.1	470.15	260.15
1,4-dioxane	-11.430	11.669	122.78	1403.5	374.15	284.15
Water	-13.742	16.684	146.02	2006.6	373.15	273.15
Triethyl amine	-11.248	8.2120	87.810	987.68	361.95	158.15
Water	-13.389	15.786	141.80	1898.6	373.15	273.15
Glycerol	-24.143	59.608	296.95	7169.2	455.15	293.15
TEGMME*	-13.638	21.245	187.36	2555.2	395.15	229.15
n-Heptane	-12.613	14.344	136.78	1725.2	371.15	182.15
Propargyl alcohol	-12.607	15.105	144.10	1816.7	387.65	220.15
Allyl alcohol	-12.866	15.305	143.07	1840.8	370.15	144.15
t-butanol	-18.476	32.029	208.50	3852.2	355.55	298.84
2-propanol	-15.032	21.950	175.63	2640.0	355.15	183.65
1-propanol	-13.415	17.792	159.51	2139.9	370.15	149.15
Bromobenzene	-13.450	16.771	149.98	2017.1	429.15	242.15
Chlorobenzene	-10.406	7.9331	91.687	954.13	405.15	228.15
Ethylbenzene	-10.807	8.5016	94.617	1022.5	409.15	178.15
Benzene	-13.254	14.955	135.71	1798.7	353.15	278.65
Dimethylsulfoxide	-10.975	11.721	128.44	1409.7	462.15	290.65
3-amino-1-propanol	-18.036	36.059	240.46	4336.9	458.65	284.15
Isoamyl alcohol	-14.322	21.640	181.72	2602.7	403.15	156.15
2-propanol	-16.403	25.430	186.46	3058.5	355.15	183.65
Ethanol	-12.997	15.680	145.10	1885.9	351.15	159.15
1,4-dioxane	-11.607	12.074	125.11	1452.2	374.15	284.15
N-methylacetamide	-13.155	19.128	174.88	2300.6	478.15	300.15
2-Methoxyethanol	-12.662	14.504	137.77	1744.4	397.65	188.15
Water	-13.307	15.568	140.70	1872.4	373.15	273.15
Propylene carbonate	-11.729	14.192	145.53	1706.9	513.15	218.15
1,2-diethoxyethane	-10.819	7.5690	84.142	910.34	394.15	199.15
Acetonitrile	-10.793	6.9895	77.885	840.64	354.65	222.15
Tetrahydrofuran	-10.393	6.7382	77.977	810.42	339.15	165.15
Methanol	-11.629	10.198	105.47	1226.5	337.75	175.55

Table 1: Arrhenius parameters of some pure liquids studied at previous works, Arrhenius activation energy E_a (kJ·mol^{-1}), the logarithm of the entropic factor of Arrhenius *ln*(*As*/Pa·s), the Arrhenius temperature (T_A /K), Arrhenius activation temperature, (*T*/K*), the melting point (T_m/K) and the boiling point (T_b/K).

Conclusion

Correlation between Arrhenius parameters reveals interesting Arrhenius temperature which is closely related to the vaporization temperature in the liquid vapor equilibrium..
We conclude that the boiling point is in causal correlation with the two viscosity Arrhenius parameters, but also implicitly in correlation with other chemical and physical properties for which there are some ones are common for the two Arrhenius parameters while others are in relationship only for only a single parameter (Ea) or (lnAs).

Reference [1] : M.A. Alkhaldi, "Estimation of boiling points by investigations of viscosity Arrhenius behaviors in Methyl Benzoate + n-Hexane binary systems at atmospheric pressure." Physics and Chemistry of Liquids . DOI: 10.1080/00319104.2017.1327582 link : http://www.tandfonline.com/doi/full/10.1080/00319104.2017.1327582