

Modeling Adiabatic Compressibility of Some Organic Liquids with Halogen Using Physico-chemical and Topological Descriptors

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ABSTRACT: The adiabatic compressibility of 15 organic halo-derivatives comprising of aliphatic and aromatic liquids have been modelled using physico-chemical parameters and topological descriptors. It has been found that the property of liquid is possible to be modelled theoretically. But physico-chemical parameters (MV, MW, ST, IR) alone are unable to do so. The topological parameters viz Wiener index and connectivity indices when added with physicochemical parameters gave excellent results. The value of regression coefficient in three-parametric model with W, and connectivity indices comes out to be 0.9434 which suggests that the model is excellent. The model is free from the defect of collinearity. The model has been tested using LOO (Cross Validated parameters) method

Keywords: Adiabatic Compressibility, QSPR, Wiener index, Connectivity indices, Topological modelling.

INTRODUCTION

In various types of liquids it is interesting to study how the density [changes](#) when the pressure is changed by a small amount. This property of liquids is described by the [compressibility](#) of the fluid—either the isothermal compressibility, β_T , or the adiabatic compressibility, β_S .

It is well known fact that when fluid is compressed, the work done on it tends to produce heat. If the heat has time to transfer to the surroundings and the temperature of the fluid remains unchanged throughout, then β_T is the relevant quantity. If the heat generated is not allowed to escape because in general the thermal conductivity of most fluids is poor, then the flow is said to be adiabatic, and β_S is needed. The study of compressibility of gases (vapors), liquids, and solids are very important as they have wide application in understanding industrial chemical processes specially, operation of heat engines and aerodynamic in automobile and aircrafts the action of an explosion and hydrodynamic effects observed during at high velocities.

The pioneer work has been done by S. Parthasarathy who has obtained the adiabatic compressibility of liquids with by the method of diffraction of light by ultra-sonic waves [1]. The adiabatic compressibility is, therefore, important property which has wide application. We thought to estimate the value for different organic liquids using mathematical models. We have already worked on the application of physico-chemical and topological indices for modeling of physical properties of drug molecules [2]. Even chemical shifts and boiling points and other important properties have been modeled successfully by V.K. Agrawal et al [3-11] using physico-chemical and topological descriptors.

With this purpose we have chosen 15 organic liquids whose adiabatic compressibilities have been experimentally measured and tried to model them using some physico-chemical and topological indices.

The structure of molecules were drawn and descriptors were calculated which are discussed in subsequent sections.

METHODOLOGY USED

The Chemsketch software from ACD labs [12] is an excellent tool for drawing of structures of molecules. This software also provides/calculates various physico-chemical parameters. The structures can be saved in the form of mol file which is further used in calculation of topological descriptors.

Topological Descriptors:

Topological descriptors are calculated from molecular graph of a molecules. These molecules are converted into graph by considering atom connections. All the carbon-hydrogen connections are suppressed i.e. hydrogen depleted graphs are considered. The details of calculation of these descriptors are described by Todeschini in his book [13].

Based on mathematical relations and distance matrices Dragon software has been designed.[14] This software calculates all kind of topological descriptors. They are presented in different groups. The researcher has a freedom to select all or some of the groups for his/her purpose.

The Hansch approach [15] has been employed for modeling the adiabatic compressibility which is based on linear relationship between property and descriptors. One can use independent descriptors for modeling. If one descriptor is used it will give mono-parametric correlation. No of independent descriptors may be used depending upon the number of data points and observing Rule of Thumb as given by Tute[16]. This rule restricts number of descriptors to one fifth as compared to data points. Meaning thereby, if the data set contains 10 molecules, then only two descriptors are allowed to be used for obtaining a correlation.

NCSS software is used for obtaining the correlation using Regression analysis [17,18].

The organic liquids taken in this study from the work of S. Parthasarthy [19] are reported in Table 1. This table also reports the experimental adiabatic compressibility values of these compounds. The physico-chemical parameters calculated by Chensketch software are presented in Table 2. The topological descriptors calculated from Dragon software are summarised in Table 3. They include Wiener [4,20], Balaban [21,22], Randic [23-25] and Kier and Hall [26,27] connectivity indices.

RESULTS AND DISCUSSION

The data mentioned above are used for regression analysis. The independent parameters are chosen from the Table 2 and 3 whereas the dependent variable is adiabatic compressibility. We also obtained a correlation matrix which shows the correlation between all the descriptors. The same is reported in Table 4.

A close look at this table reveals that:

- 1) MR is the best parameter in one-parametric model as its correlation with adiabatic compressibility is 0.9026 with a negative sign.
- 2) The other descriptors which have better potential in modelling the adiabatic compressibility are Surface tension, First order Randic connectivity index, and 3rd order Kier and Hall valence connectivity index.
- 3) Density shows very poor correlation
- 4) All other have moderate correlation

Therefore, one has to attempt for multi-parametric correlation to obtain better model. The different models tried are reported in Table 5. This table contains the values of different statistical parameters and also Pogliani's quality factor Q which is correlation of R/Se [28,29].

Now we will discuss different models as obtained after performing regression analysis[30].

One-parametric model

Out of 13 one-parametric model tried one with MR as correlating parameter gave highest value of correlation coefficient. The R² for this model comes out to be 0.7979. The model is as below:

$$AC = -1.9031(\pm 0.2656)MR + 8.8181 \quad \dots (1)$$

N=15, Se=0.1361, R²=0.7979, Adj R²=0.7979, F-ratio=51.323, Q =6.5632

In this model the coefficient of MR is negative showing that MR has negative effect towards adiabatic compressibility value for the present set of compounds.

Two-parametric model

To obtain better R²-value we tried two-parametric correlation by adding one more parameter to above model. We obtained 13 correlations with improved R² values. Two correlations have been found with MR. One with St and other with Jhetv. The only correlation out of two with MR giving better R² value comes out to be with Jhetv. The model is as below:

$$AC = -1.4450(\pm 0.2554)MR - 9.5340(\pm 3.1110)Jhetv + 8.0805 \quad \dots (2)$$

N=15, Se=0.1061, R²=0.8866, Adj R²=0.8677, F-ratio=46.922, Q = 8.8746

In the above model though the R² value shows significant improvement but another two-parametric model in which MR is missing has been found to be better than this model. This model contains Randic second order connectivity index and third order valence connectivity index. The model gave highest value of R² (0.9223). The AdjR² also shows improvement. And the Q value is also improved from 6.5632 to 10.9381. The model is as under:

$$AC = -9.0676(\pm 1.4211)\chi^2 - 9.8564(\pm 1.8025)\chi^3 + 3.2968 \quad \dots (3)$$

N=15, Se=0.0878, R²=0.9223, AdjR²=0.9094, F-ratio=71.245, Q=10.9381

The coefficients of both the parameters in above model are negative suggesting that they have retarding role towards exhibiting adiabatic compressibility.

Three-parametric model

To obtain better results we tried three-parametric correlations. Interesting MR is missing in all the models which yielded better R² values. However, ST is retained in few. The improved model having ST, Wiener index and third order connectivity index gave R² value better than two-parametric model. The R² comes out to be 0.938. Also Q value is better than the previous value. The suggested model is as follows:

$$AC = -1.0659(\pm 0.1626)ST + 0.3129(\pm 0.1338)W - 17.8311(\pm 4.8280)^3\chi + 4.777 \dots (4)$$

N=15, Se= 0.0819, R²= 0.938, Adj R²= 0.9211, F-ratio= 55.473, Q= 11.8254

In the above model the coefficients of ST and ³χ are again negative. The model is as below:

A better model is obtained when Wiener index is added to model 3 an improved statistics is resulted. The R² value changes from 0.9223 to 0.9434. Also the Q-value supports this model. The Adj R² changes significant improvement from 0.9211 to 0.9280 suggesting that W has its fare share in the model. The best three-parametric model is as given under:

$$AC = 0.1902(\pm 0.0940)W - 15.1372(\pm 3.2562)^2\chi - 8.6024(\pm 1.7225)^3\chi + 3.7697 \dots (5)$$

N=15, Se= 0.0783, R²= 0.9434, Adj R²= 0.928, F-ratio= 61.11, Q =12.4047

Randic recommendation

From the correlation matrix it is clear that some of the parameters have strong correlation. Generally such parameters are not permitted to use in combination as they may give defect of collinearity [18]. But Randic [31] believes that the parameters though interrelated may have different information. If we discard any of them the information content will also be lost. Therefore, he suggested use of these parameters together. However he suggested to check the defects by other methods. In our study we have considered the Randic recommendation. But we checked the presence of collinearity or Chance by other standard techniques.

The model is free from the defect of collinearity

The technique of calculating VIF (variance inflation factor) [32] is standard method for checking the collinearity defect. If the value of VIF is more than 10 the model suffers from the defect of collinearity.

For all the models proposed the value of VIF has been found to be less than 10 which means that proposed models are free from the defect of collinearity. In Table 8, we have reported all the values calculated for this factor for the best model.

On the basis of λ

Likewise, if Eigen values is greater than 5 then model suffers from collinearity. In all the proposed models the λ values have been found less than 5.

On the basis of condition number (k)

Another test for collinearity is condition number (k). If its value is more than 100 then the collinearity exists in the model, however, the values reported in this table shows that it is less than 100 for all the proposed models. The tolerance value (T) equal to 1 or less indicates absence of collinearity.

The Ridge trace and VIF trace also show that the proposed best model 33 (Table 5) is free from the defect of collinearity. Therefore, we conclude that the proposed model is free from any defect of collinearity and is most suitable for modelling the adiabatic compressibility of present set of compounds.

On the basis of Cross validated parameters:

Cross-validation [18,32] provides the values of PRESS, SSY, S_{PRESS}, R²_{CV} and PSE from which we can investigate the predictive power of the proposed model. It is proposed that PRESS is a good estimate of the real prediction error of the model. If it is smaller than SSY the model predicts better than chance. Under these conditions the proposed model can be considered "statistically" significant.

It is also an important observation that to be a reasonable QSPR model PRESS/SSY should be smaller than 0.4. However, the value of this ratio is smaller than 0.1 the model is accepted as an excellent model. Also, if PRESS value is transformed in a dimension less term by relating it to the initial sum of squares, we obtain R²_{CV} i.e. the complement to the traces of unexplained variance over the total variance. Thus, PRESS and R²_{CV} have good properties.

We have also calculated the cross validated parameters [24] for the proposed models which are reported in Table 6. For the best model (model 33, Table 7) the cross validated parameters comes out to be PRESS/SSY=0.06, R²_{CV}=0.94, S_{PRESS}=4.585 and PSE=3.9263. Hence, This model is having highest R²_{CV} value among all the proposed models and also all other parameters are in favour of this model. Hence this model is the best model for modeling the Ultrasonic velocity of present set of organic compounds.

To establish the above finding, we have estimated adiabatic compressibility values employing the best model (model 33, Table 5) for the compounds used in the present study. The observed and estimated values calculated are reported in Table 7. The calculated values are in good agreement with the observed values showing that the Model 33 can be used for estimated the adiabatic compressibility of present set of compounds.

To check the predictive power of the model a graph is plotted between observed and estimated values which is presented in Fig1, The quality of this model is studied with the trend line in this graph which has a R² value equal to 0.943 showing that more than 94% variance is explained by this model.

CONCLUSION

On the basis of the above we may conclude that the adiabatic compressibility of organic liquids under study can be modelled theoretically using topological and physicochemical parameters (ST, W, Connectivity indices).

Table 1: Compounds used in the present study and their Activity

Comp. No.	Name of compound	Adiabatic compressibility at 28°C, $\beta\phi \times 10^6$
1	Ethyl bromide	88.1
2	Butyl bromide	76.2
3	Butyl iodide	67.3
4	Allyl chloride	90.1
5	Acetylene dichloride(Cis)	75.4
6	AcetyleneTetracloride	48.6
7	Acetylene Tetrabromide	33.3
8	Tetrachlorethylene	58.4
9	Ortho Dichlorobenzene	49.7
10	Meta Dichlorobenzene	51.2
11	Benzoyl chloride	47.5
12	Benzyl chloride	47.8
13	Chlorobenzene	53.6
14	Bromobenzene	52.0
15	Ortho-Monochloronapthalene	39.3

Table 2 : Values of calculated physic-chemical descriptors for the compounds used in the present study

Compd. No.	MW	MR	MV	ST	D
1	108.965	19.04	74.73	23.13	1.458
2	137.018	28.31	107.73	26.03	1.271
3	184.018	33.54	113.33	29.93	1.622
4	76.524	20.52	84.53	20.03	0.905
5	96.943	21.07	77.93	25.93	1.243
6	167.849	30.62	107.83	33.93	1.556
7	343.637	41.98	107.43	60.53	3.196
8	165.833	30.45	100.33	35.63	1.653
9	147.001	36.04	113.33	36.73	1.297
10	147.001	36.04	113.33	36.73	1.297
11	140.567	36.49	115.83	39.83	1.213
12	126.58	36.01	117.13	33.83	1.08
13	112.556	31.14	101.33	33.03	1.11
14	157.007	33.94	105.63	35.43	1.486
15	162.61	48.99	135.53	42.93	1.2

Table 3 : Values of calculated topological descriptors for the compounds used in the present study

Compd. No.	W	Jhetv	$^1\chi$	$^2\chi$	$^3\chi$	$^0\chi^v$	$^1\chi^v$	$^3\chi^v$
1	4	1.898	1.414	0.707	0	3.671	2.096	0
2	20	2.302	2.414	1.354	0.707	5.085	3.096	1.048
3	20	2.365	2.414	1.354	0.707	5.657	3.5	1.25
4	10	2.297	1.914	1	0.5	3.125	1.618	0.327
5	10	2.549	1.914	1	0.5	3.422	1.643	0.429
6	29	2.993	2.643	2.488	1.333	5.69	2.952	1.714
7	29	4.675	2.643	2.488	1.333	8.856	4.178	3.857
8	29	3.676	2.643	2.488	1.333	5.536	2.518	1.286
9	60	3.135	3.805	3.239	2.54	5.577	2.961	1.58
10	61	3.078	3.788	3.377	2.199	5.577	2.955	1.257
11	88	2.854	4.305	3.642	2.593	5.429	2.932	1.219
12	64	2.832	3.932	2.912	2.302	5.228	3.066	1.306
13	42	3.021	3.394	2.743	1.894	4.521	2.478	0.985

14	42	3.155	3.394	2.743	1.894	5.351	2.893	1.262
15	140	2.913	5.377	4.617	3.933	6.675	3.888	2.066

Table 4. Correlation matrix for the inter correlation of the structural descriptors and their correlation with activity

	Adiabatic Compr.	D	MW	W	$^1\chi$	$^1\chi^v$	Jhetv	MV	$^3\chi$	$^3\chi^v$	$^0\chi^v$	$^2\chi$	ST	MR
Adiabatic Compr.	1													
D	-0.0983	1												
MW	-0.5630	0.7567	1											
W	-0.8015	-0.2554	0.2770	1										
$^1\chi$	-0.8050	-0.2554	0.2770	0.9964	1									
$^1\chi^v$	-0.6250	0.2842	0.6881	0.4421	0.4457	1								
Jhetv	-0.6036	0.4701	0.6130	0.4834	0.4870	0.2643	1							
MV	-0.7133	-0.1650	0.4126	0.8133	0.8133	0.7384	0.1541	1						
$^3\chi$	-0.7979	-0.2320	0.2896	0.9892	0.9964	0.4421	0.5085	0.8025	1					
$^3\chi^v$	-0.8286	0.3789	0.7864	0.5822	0.5966	0.7214	0.6929	0.6022	0.6002	1				
$^0\chi^v$	-0.7417	0.5599	0.9249	0.4748	0.4748	0.7846	0.5809	0.6135	0.4910	0.8686	1			
$^2\chi$	-0.7835	-0.2086	0.3022	0.9892	0.9855	0.4313	0.5229	0.7917	0.9892	0.5750	0.5072	1		
ST	-0.8883	0.2880	0.6637	0.7680	0.7680	0.5916	0.7668	0.6063	0.7842	0.7971	0.7961	0.8004	1	
MR	-0.9026	0.0519	0.5528	0.8489	0.8489	0.7060	0.5737	0.7928	0.8543	0.7328	0.7388	0.8597	0.9070	1

Table 5. Quality of statistical parameters for different models

S. No.	Parameters	Ai	B	Se	R ²	R ² Adj	F Ratio	Q= R/Se
1	D	-13.2486(±8.1647)	12.4693	0.276	0.1684	0.1045	2.633	1.1712
2	MW	-0.1771(±0.0607)	9.8691	0.2353	0.3956	0.3491	8.51	2.673
3	W	-0.3209(±0.0985)	5.4432	0.2245	0.4496	0.4073	10.62	2.9867
4	$^1\chi$	-12.1145(±2.9586)	9.5629	0.2	0.5633	0.5297	16.766	3.7527
5	$^1\chi^v$	-17.9548(±4.3380)	12.7303	0.1988	0.5686	0.5354	17.131	3.793
6	Jhetv	-19.8358(±4.6412)	13.8529	0.1952	0.5842	0.5522	18.265	3.9156
7	MV	-0.8281(±0.1905)	20.2243	0.1932	0.5925	0.5611	18.9	3.9842
8	$^3\chi$	-12.8411(±2.8454)	5.3376	0.1889	0.6104	0.5804	20.367	4.136
9	$^3\chi^v$	-15.6808(±3.1300)	4.8838	0.1768	0.6588	0.6325	25.099	4.5909
10	$^0\chi^v$	-10.1780(±1.9595)	10.6955	0.1726	0.6748	0.6498	26.981	4.7593
11	$^2\chi$	-13.0026(±2.1999)	5.8133	0.1576	0.7288	0.7079	34.933	5.4169
12	ST	-1.5643(±0.2330)	8.2666	0.1432	0.7762	0.759	45.082	6.1524

13	MR	-1.9031(\pm 0.2656)	8.8181	0.1361	0.7979	0.7823	51.323	6.5632
14	$^1\chi$	13.5815(\pm 7.5843)	8.6044	0.1457	0.786	0.7503	22.035	6.0849
	$^2\chi$	-25.2893(\pm 7.1564)						
15	W	-0.2595(\pm 0.0514)	8.1822	0.1149	0.8669	0.8447	39.081	8.1033
	Jhetv	-17.0922(\pm 2.7866)						
16	ST	-0.8116(\pm 0.3177)	7.44	0.114	0.8691	0.8473	39.833	8.1777
	MR	-1.1124(\pm 0.3812)						
17	Jhetv	-14.7872(\pm 2.7520)	12.0839	0.109	0.8804	0.8604	44.147	8.6082
	MV	-0.6217(\pm 0.1141)						
18	ST	-1.1632(\pm 0.2137)	11.3117	0.108	0.8825	0.8629	45.059	8.6983
	MV	-0.4267(\pm 0.1295)						
19	Jhetv	-9.5340(\pm 3.1110)	8.0805	0.1061	0.8866	0.8677	46.922	8.8746
	MR	-1.4450(\pm 0.2554)						
20	Jhetv	-12.0590(\pm 2.7351)	7.195	0.1014	0.8965	0.8792	51.961	9.3376
	$^2\chi$	-9.6579(\pm 1.6052)						
21	ST	-2.2547(\pm 0.2372)	5.6818	0.0984	0.9025	0.8863	55.56	9.6545
	D	17.0071(\pm 4.3119)						
22	ST	-1.1505(\pm 0.1857)	5.5874	0.096	0.9072	0.8917	58.64	9.9216
	$^3\chi$	-7.0754(\pm 1.7193)						
23	D	-13.8898(\pm 2.7365)	5.2642	0.0925	0.9138	0.8995	63.62	10.3344
	$^2\chi$	-13.1533(\pm 1.2911)						
24	MW	-0.1259(\pm 0.0242)	4.4308	0.0909	0.9167	0.9029	66.059	10.5329
	$^2\chi$	-11.3386(\pm 1.3084)						
25	ST	-1.0072(\pm 0.1886)	5.1596	0.0893	0.9197	0.9063	68.684	10.7392
	$^2\chi$	-7.4913(\pm 1.6182)						
26	$^2\chi$	-9.0676(\pm 1.4211)	3.2968	0.0878	0.9223	0.9094	71.245	10.9381
	$^3\chi^v$	-9.8564(\pm 1.8025)						
27	$^1\chi^v$	11.1963(\pm 4.7076)	10.6006	0.0917	0.9224	0.9012	43.582	10.4735
	ST	-1.5596(\pm 0.2464)						
	MV	-0.7031(\pm 0.1600)						

28	$^2\chi$	-15.0406(± 6.4522)	4.9549	0.0882	0.9282	0.9086	47.405	10.9233
	$^3\chi$	6.2876(± 6.6239)						
	$^3\chi^v$	-9.1418(± 1.9604)						
29	MW	-0.1405(± 0.0226)	3.9914	0.0854	0.9326	0.9142	50.711	11.3081
	W	0.3539(± 0.1383)						
	$^3\chi$	-23.4475(± 4.7770)						
30	MW	-0.1093(± 0.0242)	4.4092	0.0838	0.9351	0.9175	52.874	11.5394
	W	0.1801(± 0.1019)						
	$^2\chi$	-16.8318(± 3.3340)						
31	ST	-0.8765(± 0.1889)	4.9008	0.0824	0.9374	0.9204	54.949	11.7499
	W	0.1771(± 0.1002)						
	$^2\chi$	-13.3942(± 3.6560)						
32	ST	-1.0659(± 0.1626)	4.777	0.0819	0.938	0.9211	55.473	11.8254
	W	0.3129(± 0.1338)						
	$^3\chi$	-17.8311(± 4.8280)						
33	W	0.1902(± 0.0940)	3.7697	0.0783	0.9434	0.928	61.11	12.4047
	$^2\chi$	-15.1372(± 3.2562)						
	$^3\chi^v$	-8.6024(± 1.7225)						

Table 6. Cross validated parameter for the proposed models

S. No.	Parameters	PRESS/SSY	R ² CV	SPRESS	PSE
1	MR	0.2533	0.7467	7.9693	7.4191
2	$^2\chi$ $^3\chi^v$	0.0842	0.9158	5.1423	4.5994
3	ST W $^2\chi$	0.0667	0.9333	4.8199	4.1275
4	ST W $^2\chi$ W $^2\chi$ $^3\chi^v$	0.0661 0.06 0.06	0.9339 0.94	4.7985 4.585	4.1092 3.9263

Table 7. Observed and Estimated Adiabatic Compressibility for the present set of compounds using best model

Compd. No.	Obs. Adiabatic Compressibility	Est. Adiabatic Compressibility	Residual
1	88.1	88.125	-0.025

2	76.2	72.359	3.841
3	67.3	70.621	-3.321
4	90.1	82.018	8.082
5	75.4	81.14	-5.74
6	48.6	51.175	-2.575
7	33.3	32.74	0.56
8	58.4	54.857	3.543
9	49.7	46.856	2.844
10	51.2	47.735	3.465
11	47.5	49.186	-1.686
12	47.8	54.923	-7.123
13	53.6	56.059	-2.459
14	52	53.676	-1.676
15	39.3	37.03	2.27

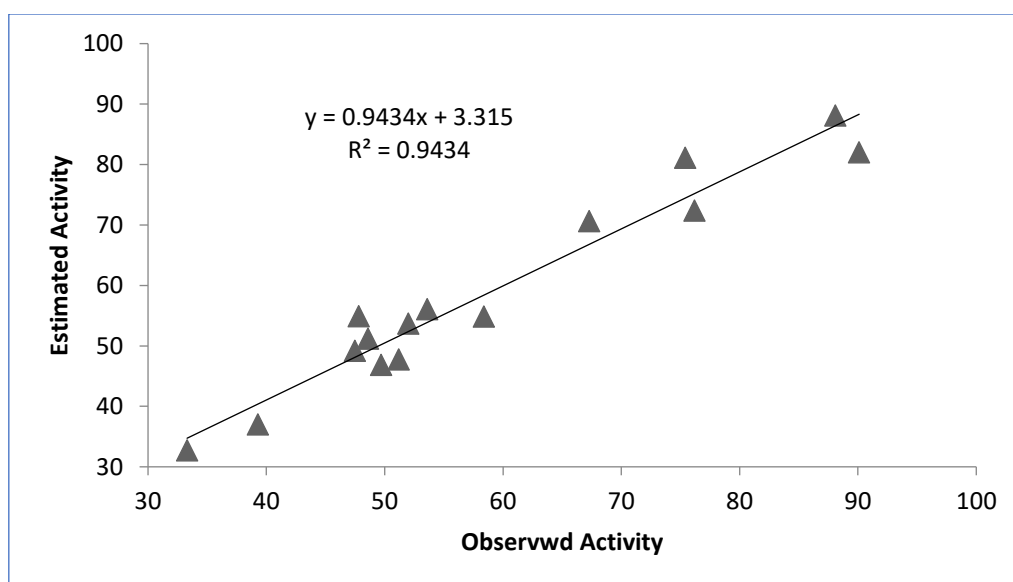


Fig 1 : Correlation between observed and estimated activity using best model

Table 8. Ridge Regression parameters for the best obtained models

Model No.	Parameters Used	VIF	T	λ_i	k
33 (Table 5)	W	7.4934	0.1334	2.2187	1.0000
	X2	8.8817	0.1126	0.7191	3.0900
	X3V	1.5448	0.6473	0.0622	35.6700

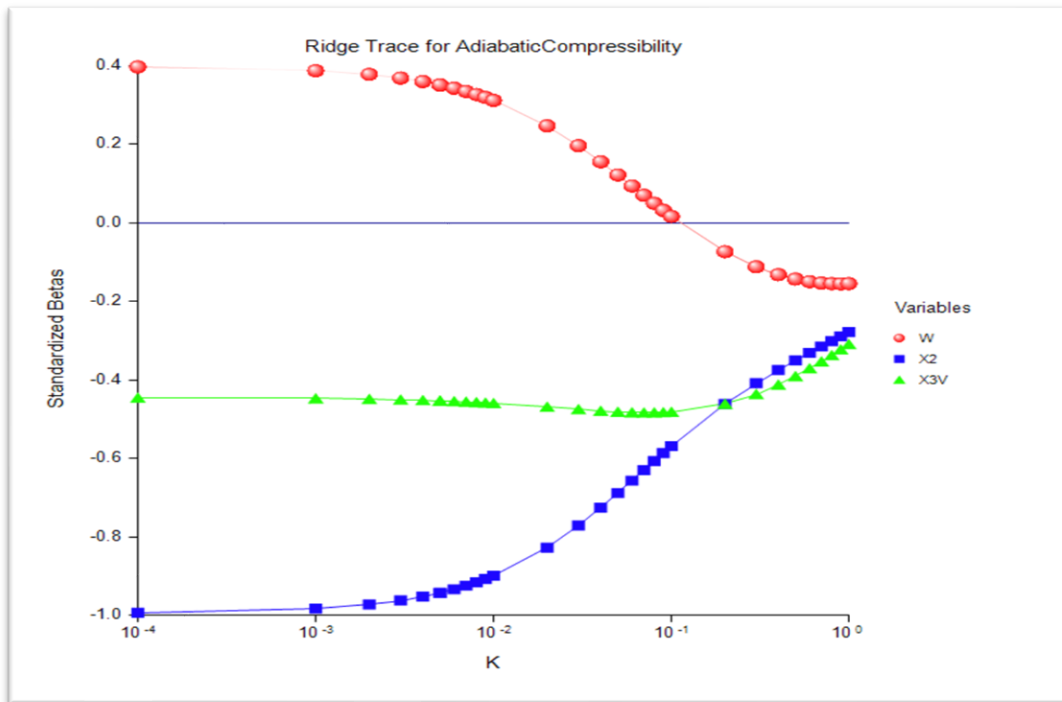


Fig. 2: Ridge plot for Adiabatic Compressibility

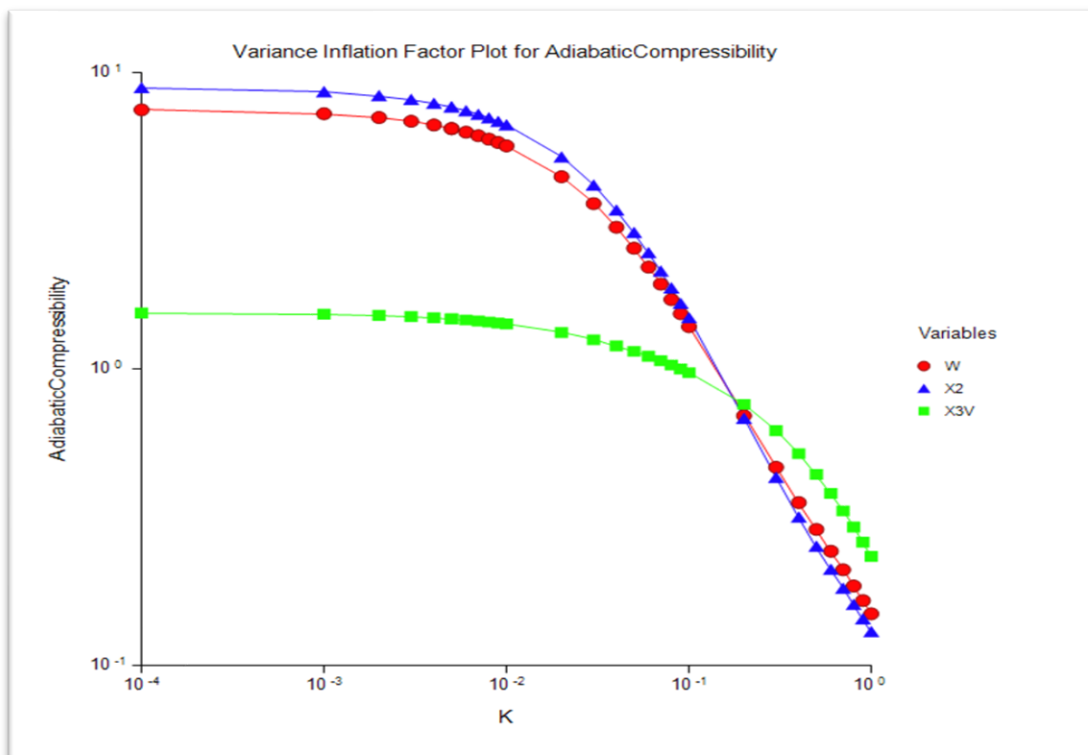


Fig. 3: Ridge plot for Adiabatic Compressibility

Availability of data

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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Conflict of Interest

The author declares that they have no known competing financial interests or personal relationship that could have appeared to influence the work reported in this paper.

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