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Melting point Models of Alkanes by using Physico-chemical Properties

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Abstract

Multivariable models were developed to predict the melting points of alkanes having 1-10 carbon atoms.The quantitative structure- property relationship (QSPR) studies have been performed on 30 compounds of a series of alkanes.The QSPR models were generated using stepwise regression analysis to determine multiple correlation coefficient and standard error. This study produced good predictive models which gave statistically significant correlations with good multiple correlation coefficient and minimum standard error using physico-chemical properties as QSPR parameters. The models were used to predict the melting points of alkanes for a set of test data from 1-10 carbon atoms for which no experimental melting point data existed.

Key-Words: Multiple correlation coefficient, MLR models, QSPR, Physico-chemical properties

Introduction

Quantitative Structure-property relationship (QSPR) is an alternative approach for estimating melting point of any compound. The premise of QSPR is that phsico-chemical properties can be correlated with molecular structure characteristics (geometric and electronic) expressed in terms of appropriate molecular descriptors [1]. QSPR studies are undoubtly of great importance in modern chemistry and pharmacy. QSPR have been traditionally developed by selecting, a priori, an analytical model (typically) linear, polynomial or lag-linear to quantity the correlation between selected molecular indices and desired physico-chemical properties, followed by regression analysis to determine model parameters [2]. The various alkanes can be characterized by their physical properties including melting points. Experimental m.p. datas are not available for all of the alkanes with $n \leq 10$. This lack of data is a motivation for constructing m.p. models which can be used to estimate the m.p. of alkanes for which no data is available [3].

Material and Methods

Alkanes

A series of 30 alkanes were selected (up to 10 carbon atom) for the present study. Then the structures of these alkanes were generated for the calculation of various physico-chemical properties by software Chem. Sketch 5.

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Calculation of physico-chemical properties [4, 5, 6]

a.Molecular Weight [MW]: It can be calculated as given below-

MW (n) = 12.01115n + 1.00797 (2n +2)

Where n denotes the number of carbons in the given alkane

b.Molar Refractivity [MR] : It can be calculated as given below-

$$MR = \frac{n-1}{n+1} \quad \frac{MW}{d}$$

Where n is the refractive index, MW = molecular weight and d = density

c.Parachor [P]:- It can be calculated as given below-

$[P] = r^{1/4} . MW/d$

Where r = surface tension

d.Index of refraction [μ] :-It can be calculated as given below-

$\mu = \text{Sin } i / \text{Sin } r$

where Sin i = sine of the angle of incidence, Sin r = sine of the angle of refraction

e.Surface tension [γ]:- It can be calculated as given below.

$\gamma = F / d$

f.Polarizability [δ]:- It can be calculated as given below.

$\delta = \mu ind/E$

Where μind = Induced dipole moment E = Electric field

g.Hydrophobic Parameter [LogP]:- It can be calculated as given below.

Log P = log compound $_{(octanol)}$ - log compound $_{(water)}$

h.Molecular surface area [S_M]:- It can be calculated as given below:

$$S_M = \sum_i S_{VW}^i - S_{OV}$$

Where S_{VW}^i - Van der Waal's area of the i-th constituent atom of a molecule

S_{OV} - Vander Waal's area of atoms inside overlapping atomic envelops

Generation of Multiple Linear Regression [MLR] models for the m.p. of alkanes with n ≤10 In this method regression analysis was done in a stepwise fashion by taking physico-chemical properties such as MW (molecular weight), MR (molar refractivity) , [P] (parachor), μ (index of refraction) , γ (surface tension) , δ (polarizability), LogP (hydrophobic parameter) and molecular surface area (S_M) (table 1) for correlation with melting point of alkanes.

a) MLR models using 1 property:-M.P v/s MW, etc
b) MLR models using 2 properties:-M.P v/s MW, MR etc
c) MLR models using 3 properties:- M.P v/s MW, MR , [P] etc
d) MLR models using 4 properties- M.P v/s MW, MR , [P] , μ etc
e) MLR models using 5 properties:- M.P v/s MW, MR , [P] , μ , γ etc
f) MLR models using 6 properties:- M.P v/s MW, MR , [P] , μ , γ , δ etc
g) MLR models using 7 properties:-M.P v/s MW, MR , [P] , μ , γ , δ , LogP etc
h) MLR models using 7 properties :-M.P v/s MW, MR , [P] , μ , γ , δ , LogP, S_M etc

Results and Discussion

In the present study the melting point models for alkanes have been generated by the help of 8 physico-chemical properties (MW, MR, [P], μ, γ, δ, LogP and S_M) using multiple linear regression methods. Total 255 MLR models were prepared out of which 8 models selected on the basis of good R values (which are more near to 1) and SE (minimum standard) are listed below:

Model no. 3: MP = - 230.757 + 0.384 * [P]
R = 0.826, SE = 20.96405, F = 59.976

Model no. 30: MP = - 601.199 + 571.011 * μ - 177.271 * S_M
R = 0.918, SE = 21.75748, F = 27.338

Model no. 52: MP = - 298.346 + 5.179 * MW + 9.678 * γ - 38.686 * □
R = 0.857, SE = 19.87560, F = 23.959

Model no. 156: MP = - 527.971 + 0.319 * [P] + 16.539 * γ – 44.917 * Log P + 91.212 * S_M R = 0.865, SE = 19.70005, F = 18.657

Model no.191: MP = - 1195.935 – 11.626 * MW + 4.329 * [P] + 24.182 * γ - 36.123 * Log P + 333.009 * S_M
R = 0.880, SE = 19.03884, F = 16.534

Model no. 239: MP = 1019.018 + 4.996 * MW – 1790.486 * μ + 41.564 * γ - 35.493 * □ 31.354 * Log P + 361.666 * S_M
R = 0.900, SE = 17.90192, F = 16.275

Model no. 251**:** MP = 679.499 – 2.469 * MW + 0.983 * [P] – 1627.061 * μ + 41.831 * γ - 30.947 * □ - 31.593 * Log P + 402.745 * S_M
R = 0.899, SE = 17.94499, F = 16.178

Model no. 255: MP = 1010.965 + 4.041 * MW – 11.223 * MR + 21.007 * [P] – 1791.101 * μ + 41.717 * γ – 159.638 * □ - 31.183 * Log P + + 363.410 * S_M
R = 0.992, SE = 6.55476, F = 16.501

Out of these models,the model 255 (with 8 physico-chemical properties) gives good value of R and less standard error and can be considered as best model for prediction of approximate melting point of any alkane for which m.p. is not present. The values obtained for m.p. from it are more close to that of experimental m.p.(table2) The results and discussion made above leads to the conclusion that QSPR study can be successfully done for predicting melting point of alkanes by using physico-chemical properties.Thus, the model 255 (with 8 physico-chemical properties) can be used for the determination of approximate melting point of any alkane having $n \leq 10$.

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Table 1: Alkanes, their experimental melting points [7] and physico-chemical properties used in present study

S/No.	Name of the Compound	Experimental M.P.	MW	MR	[P]	M	γ		Log P	S_M
1	Methane	-182.50	16.04	6.35					1.12	2.00
2	Ethane	-181.76	30.07	11.31	111.70	1.29	10.80	4.48	1.76	2.00
3	Propane	-187.60	44.10	15.94	151.50	1.33	14.10	6.32	2.28	1.83
4	Butane	-138.40	58.12	20.58	191.20	1.35	16.70	8.15	2.73	1.75
5	2-methyl propane	-159.60	58.12	20.53	188.60	1.35	15.50	8.14	2.13	1.83
6	Pentane	-129.80	72.15	25.21	231.00	1.37	18.70	9.99	3.14	1.70
7	2-methyl butane	-160.50	72.15	25.17	228.40	1.37	17.60	9.97	3.14	1.77
8	2,2-di methyl propane	-166.60	72.15	25.17	226.10	1.37	17.10	9.98	3.14	1.85
9	Hexane	-95	88.18	29.84	270.80	1.38	20.30	11.83	3.52	1.67
10	2-methyl pentane	-153	86.18	29.80	268.20	1.38	19.30	11.81	3.52	1.72
11	3-methyl pentane	-118	86.18	29.80	268.20	1.38	19.30	11.81	3.52	1.72
12	2,2-di methyl butane	-98.8	86.18	29.81	265.90	1.38	18.80	11.81	3.52	1.79
13	2,3-di methyl butane	-128	86.18	29.76	265.60	1.38	18.30	11.79	3.52	1.79
14	Heptane	-91	100.20	34.47	310.60	1.39	21.60	13.66	3.87	1.64
15	3-ethyl pentane	-118.6	100.20	34.43	308.00	1.39	20.60	13.65	3.87	1.69
16	2,2-di methyl pentane	-123.8	100.20	34.44	305.70	1.39	20.20	13.65	3.87	1.74
17	2,3-di methyl pentane	-135	100.20	34.39	305.40	1.39	19.70	13.63	3.87	1.74
18	2,4-di methyl pentane	-123	100.20	34.39	305.40	1.39	S19.70	13.63	3.87	1.74
19	2- methyl hexane	-118	100.20	34.43	308.00	1.39	20.60	13.65	3.87	1.69
20	3-methyl hexane	-119	100.20	34.43	308.00	1.39	20.60	13.65	3.87	1.69
21	Octane	-57	114.23	39.11	350.40	1.40	22.60	15.50	4.20	1.61
22	3-methyl heptane	-121	114.23	39.07	347.80	1.40	21.80	15.48	4.20	1.63
23	2,2,3,3-tetra methyl butane	-95.5	114.23	39.04	340.60	1.40	20.10	15.47	4.20	1.81
24	2,3,3-tri methyl pentane	-100.7	114.23	39.03	342.90	1.40	20.50	15.47	4.20	1.76
25	2,3,4-tri methyl pentane	-110	114.23	38.98	342.50	1.40	20.10	15.45	4.20	1.75
26	2,2,4-tri methyl pentane	-107.38	114.23	39.03	342.90	1.40	20.50	15.47	4.20	1.76
27	Nonane	-53	128.26	43.74	390.20	1.41	23.50	17.34	4.52	1.59
28	2-methyl octane	-80	128.26	43.70	387.60	1.41	22.70	17.32	4.52	1.62

29	Decane	243.7	142.28	48.37	430.00	1.41	24.30	19.17	4.82	1.56
30	2-methyl nonane	198.6	142.28	48.33	427.30	1.41	23.50	19.16	4.82	1.59

Table 2: The Experimental m.p. and calculated m.p. by the good MLR models for all the experimental alkanes

S/No.	Exp. MP	Calculated MP with good models							
		Model No. 3	**Model No. 30**	**Model No. 52**	**Model No. 156**	**Model No. 191**	**Model No. 239**	**Model No. 251**	**Model No. 255**
1	-182.50	-118.50	-173.28	-182.69	-176.94	-181.31	-182.58	-182.58	-182.54
2	-181.76	-190.04	-219.81	-211.42	-208.43	-211.89	-182.49	-182.49	-182.47
3	-187.60	-174.77	-165.33	-177.26	-171.69	-179.21	-189.96	-189.96	-189.90
4	-138.40	-159.54	-139.10	-150.06	-147.21	-151.94	-155.39	-155.39	-155.53
5	-159.60	-160.54	-155.39	-162.03	-167.05	-144.58	-157.11	-157.11	-157.25
6	-129.80	-144.28	-118.99	-128.93	-128.31	-130.51	-134.96	-133.96	-134.21
7	-160.50	-145.27	-133.24	-139.83	-139.23	-142.46	-154.11	-154.11	-154.15
8	-166.60	-146.16	-149.53	-144.90	-149.01	-146.94	-145.90	-145.90	-146.08
9	-95	-129.01	-107.91	-110.16	-113.19	-108.97	-96.87	-96.87	-95.28
10	-153	-130.01	-118.09	-121.70	-121.78	-123.75	-126.41	-126.41	-126.50
11	-118	-130.01	-118.09	-121.70	-121.78	-123.75	-126.41	-126.41	-126.50
12	-98.8	-130.89	-132.34	-126.71	-130.57	-128.34	-121.67	-121.67	-121.89
13	-128	-131.00	-132.34	-131.61	-132.35	-134.46	-142.34	-142.34	-142.25
14	-91	-113.74	-96.84	-97.63	-99.50	-97.91	-83.75	-83.75	-84.10
15	-118.6	-114.74	-107.02	-107.59	-108.10	-108.83	-107.27	-107.27	-107.38
16	-123.8	-115.62	-117.20	-111.60	-114.55	-112.37	-105.70	-105.70	-105.89
17	-135	-115.74	-117.20	-116.49	-116.33	-118.49	-126.37	-126.37	-126.25
18	-123	-115.74	-117.20	-116.49	-116.33	-118.49	-126.37	-126.37	-126.25
19	-118	-114.74	-107.02	-107.59	-108.10	-108.83	-107.27	-107.27	-107.38
20	-119	-114.74	-107.02	-107.59	-108.10	-108.83	-107.27	-107.27	-107.38
21	-57	-98.47	-85.76	-86.51	-87.13	-86.04	-76.60	-76.60	-76.90
22	-121	-99.47	-89.83	-94.41	-92.05	-94.76	-102.55	-102.55	-102.54
23	-95.5	-102.23	-126.48	-111.39	-116.17	-111.20	-107.63	-107.63	-107.67
24	-100.7	-101.35	-116.30	-107.38	-109.71	-107.66	-109.20	-109.20	-109.16
25	-110	-101.50	-114.27	-111.28	-110.16	-112.60	-129.34	-129.34	-128.99
26	-107.38	-101.35	-116.30	-107.38	-109.71	-107.66	-109.20	-109.20	-109.16
27	-53	-83.21	-76.72	-76.40	-76.23	-74.96	-69.66	-69.66	-69.88
28	-80	-84.20	-82.83	-84.30	-82.14	-83.59	-91.92	-91.92	-91.88
29	-29.7	-67.94	-70.62	-67.23	-64.95	-64.58	-51.84	-51.84	-51.97
30	-74.4	-68.97	-76.72	-75.19	-70.86	-73.16	-74.30	-74.30	-74.17

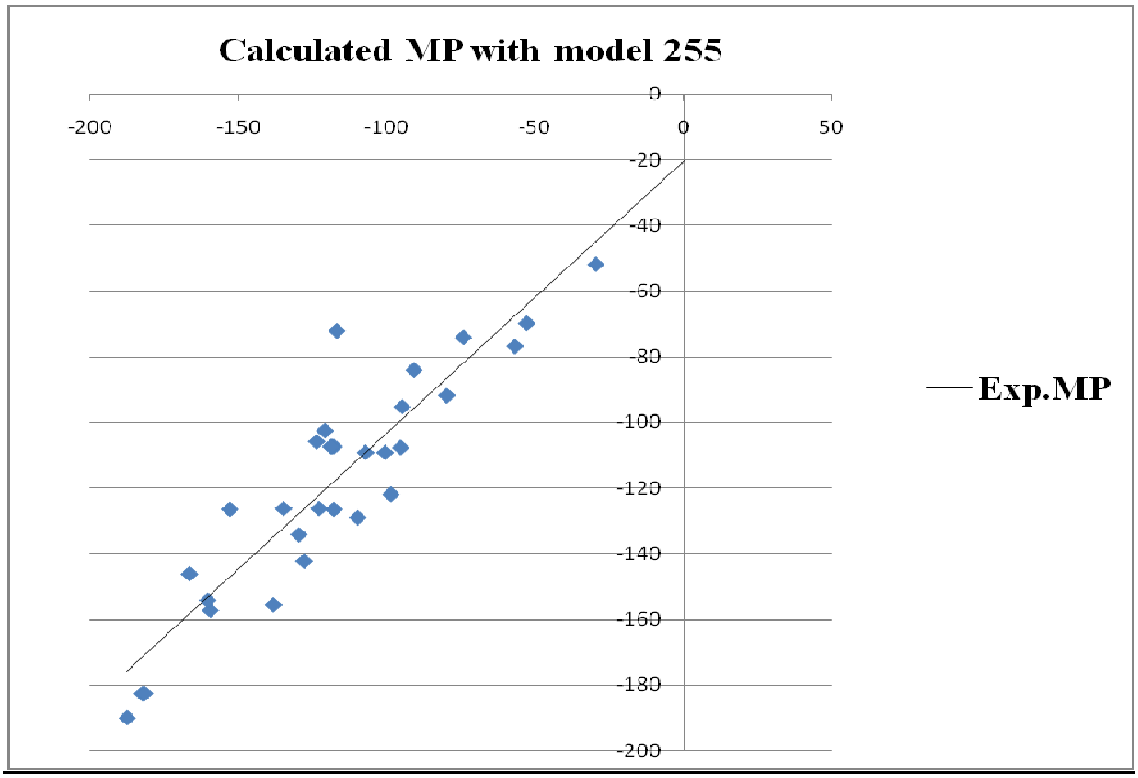

Fig. 1: Experimental melting points v/s calculated melting points using model no.255 (with physico-chemical properties)

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