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Research paper

Prediction of Ignition Delay Times for Amine-based Liquid Propellants through a QSPR Approach

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Abstract: Decreasing the ignition delay time in the combustion chamber of a rocket engine is required from a safety point of view. However it takes a lot of time and money to find the most suitable compounds with a low ignition delay time. In the present research, a model is proposed to predict the ignition delay time of amine-based liquid propellants through the quantitative structure-property relationship (QSPR) method. This model was derived based on 35 data sets collected from reliable references and by the selection of appropriate descriptors using multivariate linear regression (MLR). The determination coefficient, mean absolute deviation and root mean square deviation of the new model were 0.9901, 2.51 and 3.19 ms, respectively, which indicates high reliability. Furthermore, the values of the cross validation coefficients of the new proposed model were Q^2_{LOO} = 0.9903 and Q^2_{LMO} = 0.9906, which confirm its sufficient validation. The most important variables which have an effect on the ignition delay time of amine-based liquid propellants were identified as the elemental composition, temperature and the percentage ratio of oxidizer to fuel (*O/F*).

Keywords: ignition delay time, amine-based liquid propellants, QSPR, multivariate linear regression method

1 Introduction

In one category, propellants are divided into solid and liquid classifications. Furthermore, liquid propellants are divided into two general categories according to their components: bipropellants (two-component propellants such as kerosene as fuel and hydrogen peroxide (H_2O_2) as oxidizer) and monopropellants (single-component propellants such as H_2O_2) [1]. Some fuels, such as monomethylhydrazine (MMDH), ignite spontaneously after mixing with oxidizers such as nitric acid (HNO_3). A propellant whose fuel and oxidizer have this characteristic is called a self-igniting propellant [1].

In such fuels, the time that passes from the initial contact of the fuel and the oxidizer to the advent of the flame is called the reaction ignition delay time [2]. By testing different sorts of fuel and oxidizer, researchers have searched to find propellants with the lowest ignition delay time, such as propellants with MMDH and dimethylhydrazine (DMH) fuel. But due to the toxicity and carcinogenicity of these fuels, their utilization has been restricted [3].

Considering that the synthesis of new fuels and experimental testing occupies a lot of time and is not economically viable, obtaining theoretical models to estimate the properties of propellants that have not yet reached the synthesis and testing stages is urgently required. By reviewing the available researches, various theoretical models have been introduced to predict the physico-chemical properties of chemical compounds, especially propellants, and some of these researches are mentioned below.

In 2017, Guangjing Yu *et al.* [4] investigated the ignition delay and linear burning of a gas-to-liquid (GTL) fuel obtained from the Fischer-Tropsch process. They investigated the ignition delay of this fuel using a detailed kinetic model. The prediction made by this model was consistent with the reported values. It was observed that the data from this model showed better agreement with the mechanism [4]. Guangjing Yu *et al.* [5] conducted another study in 2018 on the ignition delay time and the linear burning rate on JP-8 fuel. They simulated the addition of syngas to JP-8 fuel in Contra software and concluded that mixing syngas with JP-8 reduces the ignition delay time and increases the linear burning speed [5]. Mohammadi and Gorji [6] predicted the shelf life of amine based liquid rocket propellants using the Arrhenius equation. According to their kinetic studies, the shelf life of an amine based rocket propellant depends highly on the initial and final concentration of triethylamine and the oxidation reaction of triethylamine was a zero order reaction.

In research on kerosene hydrocarbons, Zohari and Ebrahimzadeh [7], in 2017 investigated the relationship between the flash point of these compounds and

their molecular structure by means of a multiple linear regression approach. They reported that the flash point of hydrocarbons that make up kerosene is a function of several molecular descriptors and structural parameters. The validation tests of the proposed method verified that their model is highly predictive [7]. In 2019, in another report, Zohari *et al.* [8] performed research on predicting the ignition delay time of 31 self-igniting derivatives of an imidazolium ionic liquid with white fuming nitric acid oxidizer, by QSPR modelling.

There are different methods for predicting the properties of materials with both advantages and restrictions. The method chosen in the present research to predict and present the model is the QSPR approach (Quantitative Structure-Property Relationship). This method is based on exploring a quantitative relationship between structure and various features [9-11]. After examining the structure and characteristics of amine-based liquid propellants and finding their relationship with the ignition delay time, a model is presented to predict the ignition delay time of this class of propellants.

In order to collect data, articles in which the ignition delay time of the amine liquid fuels was performed by the drop test or cup test were reviewed. Many articles were available in this field, but considering the importance of reporting the oxidizer/fuel (*O/F*) ratio, the number of usable data was very limited. Consequently, the data were extracted from four sources: Pakdehi and Shirzadi [3], Durgapal *et al.* [12, 13] and Ladanyi and Miller [14].

2 Materials and Methods

2.1 Calculation and model building

With the help of the collected data, a relationship between the ignition delay time of amine-based liquid propellants and their structural characteristics was obtained in this research. The multiple linear regression method has been used to derive this model. In order to obtain the desired correlation between the ignition delay time and the molecular structure of amine-based liquid propellants it is vital to investigate various molecular descriptors. A molecular descriptor can convert a molecular characteristic to a numerical variable. Furthermore, a step-by-step method *via* utilization of the SPSS software has been used to enter the calculated descriptors into the model.The two-dimensional structures of the fuel and oxidizers in the collected data used in the ignition delay tests were drawn through Chemdraw software and optimized by MM2 molecular mechanics force field. The most valid correlation was obtained by applying the most significant descriptors on the ignition delay time of a training set. Subsequently, the

determination coefficient verifies the reliability of the model, and cross validation strategies were used to analyze its predictive ability. Afterwards, the introduced model was tested for some amine-based liquid propellants as a test set.

After applying linear regression on the final descriptors, along with two structural modification parameters (which had positive and negative contributions to the amount of the ignition delay time), it was feasible to gain the best correlation, Equation 1, by an amalgamation of elemental composition, the ratio of oxidizer to fuel, as well as several non-additive structural parameters.

$$ID = 21.04 - 7.60\,\frac{O}{F} + 18.00\,n_{CH_2} - 0.26\,Tn_H + 0.82\,Tn_N + 38.78\,ID^+ - 29.83\,ID^- \quad (1)$$

where n_{CH_2} is the number of CH_2 molecular components, T is the temperature in degrees centigrade, n_H is the number of hydrogen atoms, n_N is the number of nitrogen atoms, and O/F is the percentage ratio by weight of oxidizer to fuel. In addition, according to the data in Table 1, ID^+ is a correction parameter with a positive effect and ID^- is a correction parameter with a negative effect (during ignition delay). The method of least squares of residuals was used in calculating the correction parameters. To find the coefficient values of the variables in the least-squares manner, the left-division method was used for solving linear equations when the equation set is over determined [15]. Based on the final model, the descriptors CH_2, $T*n_H$, $T*n_N$ and O/F, and the two structural correction parameters ID^+ and ID^- (for positive and negative ignition delay deviations in the initial model, respectively) were calculated. Finally a model with 6 variables was obtained. The correlation matrix of the descriptors is given in Table 2. As can be seen, the descriptors have low and favorable correlations.

Table 1. Definition of increasing (ID^+) and decreasing (ID^-) correction factors

Non-additive structural parameter	ID^+	ID^-
UDMH/ WFNA, *O/F* = 4.5 UDMH/SNA Hydrazine/WFNA Cumene:UDMH/RFNA DMAZ/AK27	0.50	–
Hydrazine/H_2O_2, with temperature above 5 °C UDMH/HNO_3 Cumene:UDMH(70/30)/RFNA	0.15	
DMAZ/WFNA Triethylamine/HNO_3	1.10	
n-Heptane:UDMH (70:30)/RFNA, *O/F* = 3.0 Isooctane:UDMH (70:30)/RFNA	1.75	
n-Heptane:UDMH (70:30)/RFNA, *O/F* = 5.0 Isooctane:UDMH (60:40)/RFNA, *O/F* = 3.0 UDMH/RFNA, *O/F* = 1.5	–	0.45
n-Heptane:UDMH (70:30)/RFNA, *O/F* = 3.0 MMH/N_2O_4		1.10
Hydrazine:UDMH (50:50)/N_2O_4		1.20
UDMH/N_2O_4		0.80

Table 2. The correlation matrix of variables in Equation 1

Descriptor	*O/F*	n_{CH_2}	*T*nH*	*T*nN*	ID^+	ID^-
O/F	1					
n_{CH_2}	–0.0922	1				
*T*nH*	–0.6308	0.4429	1			
*T*nN*	0.0567	–0.3579	–0.0561	1		
ID^+	–0.0287	0.3212	0.1340	–0.0194	1	
ID^-	0.0449	–0.0461	–0.1269	0.3564	–0.2481	1

Table 3. Comparison of the predicted ignition delay time of amine-based liquid propellants (ID_C) with experimental data (ID_E) and their percentage of relative errors (RE) as a training set

No	Fuel	Oxidizer	O/F	ID_E	ID_C	RE [%]
1	UDMH	RFNA	1.50	3.60	2.94	18.25
2	UDMH	WFNA	3.00	9.80	8.27	15.66
3	UDMH	WFNA	4.50	9.70	18.93	95.10
4	UDMH	SNA	1.50	9.00	11.37	26.34
5	UDMH	SNA	3.00	8.90	5.23	41.20
6	UDMH	Mixed Acid[a)]	3.00	9.00	5.77	35.86
7	n-Heptane-UDMH (70/30)	RFNA	3.00	122.00	127.28	4.33
8	n-Heptane-UDMH (70/30)	RFNA	5.00	56.00	52.86	5.61
9	n-Heptane-UDMH (60/40)	RFNA	3.00	24.00	19.76	17.67
10	n-Heptane-UDMH (60/40)	RFNA	5.00	30.00	31.87	6.24
11	Isooctane-UDMH (70/30)	RFNA	3.00	121.00	114.92	5.02
12	Isooctane-UDMH (60/40)	RFNA	5.00	36.00	34.63	3.80
13	Cumene-UDMH (70/30)	RFNA	3.00	14.00	9.15	34.65
14	Cumene-UDMH (70/30)	RFNA	5.00	15.00	13.86	7.61
15	Cumene-UDMH (60/40)	RFNA	3.00	9.00	4.50	50.05
16	Cumene-UDMH (60/40)	RFNA	5.00	11.00	14.63	33.04
17	Triethylamine	HNO_3	0.25	68.66	67.49	1.70
18	Triethylamine	HNO_3 and 8.35 wt.% NTO[b)]	0.25	23.66	25.15	6.30
19	Triethylamine	HNO_3 and 15.23 wt.% NTO	0.25	23.52	25.41	8.04
20	Triethylamine	HNO_3 and 21.30 wt.% NTO	0.25	23.33	25.64	9.91
21	UDMH	HNO_3	4.00	4.83	8.15	68.66
22	UDMH	HNO_3 and 8.35 wt.% NTO	4.00	4.70	3.59	23.52
23	UDMH	HNO_3 and 15.23 wt.% NTO	4.00	4.40	4.64	5.38
24	UDMH	HNO3 and 21.30 wt.% NTO	4.00	4.20	3.47	17.38
25	DMAZ	NTO	2.60	68.00	73.58	8.21
26	DMAZ	AK27	2.78	83.00	80.59	2.90
27	UDMH	NTO	3	2.00	3.12	55.88
28	Aerozine 50	NTO	2.24	1.50	3.30	120.03
29	MMH	NTO	2.48	1.00	2.27	126.51
30	Hydrazine	WFNA	1.19	57.00	57.47	0.83
31	Hydrazine	WFNA	1.19	59.00	55.57	5.82
32	Hydrazine	H_2O_2	1.56	8.00	8.97	12.08
33	Hydrazine	WFNA	1.25	58.00	57.52	0.82
34	Hydrazine	H_2O_2	1.53	11.00	10.83	1.58
35	Hydrazine	H_2O_2	1.53	8.00	9.07	13.38

[a)] Ref. [7], [b)] Ref. [8]

3 Results and Discussion

3.1 Independent variables with increasing/decreasing functions

There are four cases:

1. Increasing the *O/F* ratio, to an optimal extent, reduces the ignition delay time.
2. Increasing the molecular component of CH_2 has a significant effect on increasing the ignition delay time. The results obtained showed that in these cases, increasing the *O/F* ratio can cause a decrease in the ignition delay time.
3. Increasing the temperature and the number of propellant hydrogen atoms simultaneously has a low influence on reducing the ignition delay time.
4. Increasing the number of propellant nitrogen atoms and increasing the temperature, or increasing each of these alone, is insignificant in increasing the ignition delay time, but compared to case 3, it has a greater effect on the ignition delay time.

3.2 Reliability and model validation

According to the regression analysis on the training set, the desired statistical parameters were obtained and are presented in Table 4.

Table 4. Statistical coefficients of regression analysis on the training set

Regression statistics	
Multiple *R*	0.995
R^2	0.990
Adjusted R^2	0.988
Standard error	3.568
Observations	35

According to Table 4, it can be seen that the correlation coefficient, with a value of 0.995, demonstrates a good linear relationship between the descriptors and the ignition delay time. Based on the same table, the value of the coefficient of determination shows, up to 99%, that the changes in the ignition delay time are explained by the descriptors. This high value confirms the high predictive power of the model. Furthermore, the adjusted coefficient of determination, with a value of 0.988, shows that all of the descriptors participating in the model have a role in the changes to the ignition delay time. The standard error of 3.568 also shows the favorable proximity of the defining points of the experimental ignition delay time with the model prediction line. In order to validate the model obtained from the training set, firstly the coefficient of determination (R^2) and

the adjusted coefficient of determination were obtained. According to Table 4, the value of R^2 was 0.990 and the adjusted coefficient of determination was 0.988, indicating the high validity and reliability of the model since the value of R^2 is very close to 1 and also has a slight variation with the adjusted coefficient of determination. It is noteworthy that the average absolute deviation and root mean square deviation for the training set were 2.51 and 3.19, respectively. The statistical parameters of Equation 1, which permit the relative weights of the variables in the proposed model to be determined, are listed in Table 5. The statistical parameter and standard error were used to measure the accuracy with which a sample is representative of the population. The parameter, *P*-value, represents the importance of an observed variation. If the *P*-value is less than 0.05, it verifies that the observed variation due to the variable is not random and indicates a significant effect on the model. In consequence, the desirable statistical parameters and R^2 value confirm that the calculated results are consistent with the experimental data.

Table 5. Standardized coefficients and some statistical parameters of Equation 1

	Coefficient	Standard error	*P*-value	Lower 95%	Upper 95%
Intercept	21.04	3.15	2.92×10^{-7}	14.60	27.48
O/F	–7.60	0.56	8.38×10^{-14}	–8.75	–6.45
n_{CH_2}	18.00	0.60	9.35×10^{-23}	16.76	19.23
T^*n_H	–0.26	0.02	2.9×10^{-16}	–0.30	–0.23
T^*n_N	0.82	0.04	5.56×10^{-18}	0.74	0.91
ID^+	38.78	1.51	5.03×10^{-21}	35.69	41.87
ID^-	–29.83	2.02	9.22×10^{15}	–33.96	–33.70

In further research, cross-validation was performed by means of leave-many-out (LMO) and leave-one-out (LOO) methods. In the LMO method, 7 data were randomly removed from the total of 35 in the training data set, and regression analysis was performed on the remaining data. According to the results of this analysis the averaging of the R^2 coefficient, defined as Q^2, was performed from the 5 steps of the regression calculation. The average Q^2 was equal to 0.9906, which is very close to R^2 and indicates the high predictive power of the model. In the LOO method, each time one of the 35 in the training data was removed, and after removal regression analysis was performed, and the R^2 value of each step was calculated and eventually averaged. A mean value of 0.9903 was obtained once again, confirming the good predictability of the model.

By presenting the model to the test set, Table 6, external validation was

performed and by calculating the average absolute deviation and also the root mean square deviation for this set, values of 2.91 and 3.47 were obtained, respectively. The proximity of these values with the same values from the training set, verifies the high reliability and predictability of the model.

Table 6. Comparison of predicted ignition delay time with computational data as a test set

No	Fuel	Oxidizer	*O/F*	ID_E	ID_C	*RE* [%]
1	UDMH	RFNA	3.00	6.40	11.48	79.33
2	UDMH	RFNA	4.50	6.00	3.04	49.33
3	UDMH	WFNA	1.50	9.30	13.80	48.34
4	UDMH	SNA	4.50	11.40	15.62	37.00
5	Isooctane-UDMH (60/40)	RFNA	3.00	34.00	28.56	16.01
6	Triethylamine	HNO_3 and 1.97 wt.% NTO	0.25	24.66	24.91	1.01
7	UDMH	HNO_3 and 1.97 wt.% NTO	4.00	4.76	2.63	44.79
8	DMAZ	WFNA	2.86	95.00	96.34	1.41
9	Hydrazine	H_2O_2	1.56	11.00	10.74	2.36

By examining the statistical parameters of the training set, it was found that all of the parameters confirmed the high reliability of the model. In order to evaluate the value of Q^2 of internal validation and for better indicating the power of predictability, Roy *et al.* [16] reported two statistical parameters as and , which are defined in Equations 2-5.

$$\overline{r_m^2} = \frac{(r_m^2 + r_m'^2)}{2} \tag{2}$$

$$\Delta r_m^2 = |r_m^2 - r_m'^2| \tag{3}$$

$$r_m^2 = r^2 \times \left(1 - \sqrt{(r^2 - r_0^2)}\right) \tag{4}$$

$$r_m'^2 = r^2 \times \left(1 - \sqrt{(r^2 - r_0'^2)}\right) \tag{5}$$

where r^2 and r_0^2 are the squared correlation coefficients between the cross validation estimated results and experimental data, with and without intercept,

respectively. The parameter of $r_0'^2$ has the same concept of r_0^2, but uses the reversed axes. Roy *et al.* [16] claimed that for a model with a desirable power of predictability, the value of Δr_m^2 should be less than 0.2 and r_m^2 should be more than 0.5. As can be seen in the Table 7, the values of Δr_m^2 and r_m^2 are 0.01 and 0.97, respectively.

Table 7 illustrates the reliability and validation outcomes of this regression model and confirms that there is little difference between Q^2_{LOO}, Q^2_{LMO}, Q^2_{EXT} and R^2 of Equation 1. Consequently, the proposed correlation is a perfect model and has good predictive power. Figure 1 is drawn based on the experimental and predicted values of the two training and test sets, revealing the relationship between predicted and experimental ignition delay times.

Table 7. Validation test results of the regression model obtained

Parameter	R^2	Q^2_{EXT}	Q^2_{LOO}	Q^2_{LMO}	*RMSD* [ms]	*AAD* [ms]	r_m^2	Δr_m^2
Equation 1	0.9901	0.9973	0.9903	0.9906	3.19	2.51	0.97	0.01

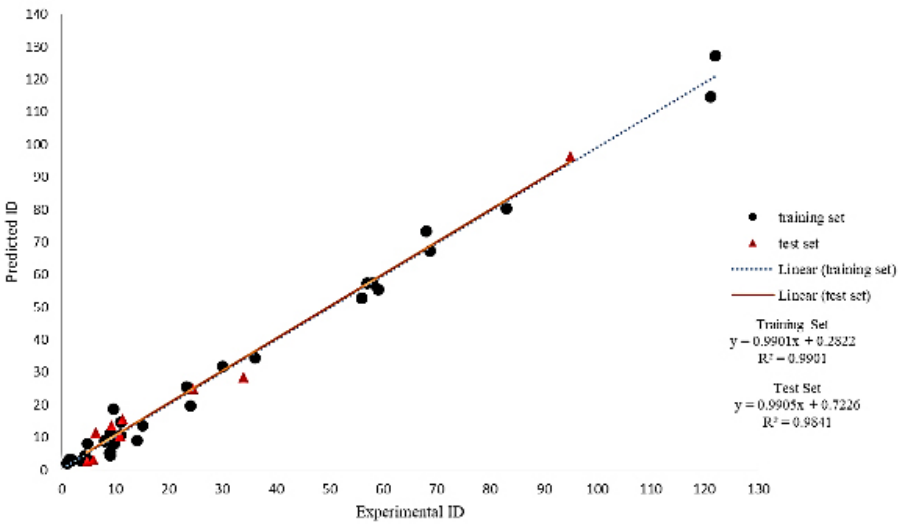

Figure 1. Predicted ignition delay time of amine-based liquid propellants vs experimental data for both training and test sets.

4 Conclusions

- In this study, a reliable correlation was obtained between the ignition delay time of amine-based liquid propellants and their molecular structures. The correlation obtained demonstrates the ability to predict the ignition delay time of amine-based liquid propellants using structural descriptors including: CH_2, *T*nH*, *T*nN*, *O/F* and two structural parameters.
- According to the satisfactory statistical results of the model ($R^2 = 0.9901$, $Q^2_{LOO} = 0.9903$ and $Q^2_{LMO} = 0.9906$), the model shows good performance for predicting the ignition delay time of amine-based liquid propellants. Also, the mean absolute deviation and root mean square deviation of the new model are 2.51 and 3.19 ms, respectively, which shown that it is highly reliable.
- It is expected that the use of this model will lead to the design of more efficient propellants in terms of optimal ignition delay time.

References

[1] Guseinov, S.L.; Fedorov, S.G.; Kosykh, V.A.; Storozhenko, P.A. Hypergolic Propellants Based on Hydrogen Peroxide and Organic Compounds: Historical Aspect and Current State. *Russ. Chem. Bull.* **2018**, *67*(11): 1943-1954; https://doi.org/10.1007/s11172-018-2314-1.

[2] Hampton, C.S.; Ramesh, K.K.; Smith, J.E. Importance of Chemical Delay Time in Understanding Hypergolic Ignition Behaviors. *Proc. 41st Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, **2003**.

[3] Pakdehi, S.G.; Shirzadi, B. Specific Impulse and Ignition Delay Time Assessment for DMAZ with Liquid Oxidizers for an Upper Stage Rocket Engine. *Iran. J. Chem. Chem. Eng.* **2017**, *36*(6): 171-176; https://doi.org/10.30492/ijcce.2017.26594.

[4] Yu, G.; Askari, O.; Hadi, F.; Wang, Z.; Metghalchi, H.; Kannaiyan, K.; Sadr, R. Theoretical Prediction of Laminar Burning Speed and Ignition Delay Time of Gas-to-Liquid Fuel. *J. Energy Resour. Technol.* **2017**, *139*(2): 022202-022208; https://doi.org/10.1115/1.4033984.

[5] Yu, G.; Askari, O.; Metghalchi, H. Theoretical Prediction of the Effect of Blending JP-8 with Syngas on the Ignition Delay Time and Laminar Burning Speed. *J. Energy Resour. Technol.* **2018**, *140*(1): 012204-012209; https://doi.org/10.1115/1.4037376.

[6] Mohammadi, K.; Gorji, M. Prediction of Amine-Based Liquid Rocket Propellant Shelf Life. *Propellants Explos. Pyrotech.* **2013**, *38*(4): 541-546; https://doi.org/10.1002/prep.201200091.

[7] Zohari, N.; Ebrahimzadeh Qhomi, M.M. Two Reliable Simple Relationships between Flash Points of Hydrocarbon Kerosene Fuels and Their Molecular Structures. *Z. Anorg. Allg. Chem.* **2017**, *643*(15): 985-992; https://doi.org/10.1002/zaac.201700142.

[8] Fareghi-Alamdari, R.; Zohari, N.; Sheibani, N. Reliable Evaluation of Ignition Delay Time of Imidazolium Ionic Liquids as Green Hypergolic Propellants by a Novel Theoretical Approach. *Propellants Explos. Pyrotech.* **2019**, *44*(9): 1147-1153; https://doi.org/10.1002/prep.201800343.
[9] Zohari, N.; Montazeri, M.; Hosseini, S.G. Estimation of the Detonation Pressure of Co-crystal Explosives through a Novel, Simple and Reliable Model. *Cent. Eur. J. Energ. Mater.* **2020**, *17*(4): 492-505; https://doi.org/10.22211/cejem/131687.
[10] Zohari, N.; Mohammadkhani, F.G. Detonation Velocity Assessment of Energetic Cocrystals Using QSPR Approach. *Z. Anorg. Allg. Chem.* **2020**, *646*(1): 30-35; https://doi.org/10.1002/zaac.201900202.
[11] Zohari, N.; Abrishami, F.; Zeynali, V. Prediction of Decomposition Temperature of Azole-based Energetic Compounds in Order to Assess of Their Thermal Stability. *J. Therm. Anal. Calorim,* **2020**, *141*: 1453-1463; https://doi.org/10.1007/s10973-019-09127-2.
[12] Durgapal, U.C.; Dutta, P.K.; Pant, G.C.; Ingalgaonkar, M.B.; Oka, V.Y.; Umap, B.B. Studies on Hypergolicity of Several Liquid Fuels with Fuming Nitric Acids as Oxidizers. *Propellants Explos. Pyrotech.* **1987**, *12*(5): 149-153; https://doi.org/10.1002/prep.19870120503.
[13] Durgapal, U.C.; Venugopal, V.K. Hypergolic Ignition of Rocket Propellants with Nitric Acid Containing Dissolved Nitrogen Tetroxide. *AIAA J.* **1974**, *12*(11): 1611-1612; https://doi.org/10.2514/3.49561.
[14] Ladanyi, D.J.; Miller, R.O. *Comparison of Ignition Delays of Several Propellant Combinations Obtained with Modified Open-cup and Small-scale Rocket Propellant Apparatus.* NACA Research Memorandum E53D03, US, **1953**.
[15] Palm, W.J. *Introduction to Matlab for Engineers.* 3rd Ed., McGraw-Hill, New York, **2010**.
[16] Pratim Roy, P.; Paul, S.; Mitra, I.; Roy, K. On Two Novel Parameters for Validation of Predictive QSAR Models. *Molecules* **2009**, *14*: 1660-1701; https://doi.org/10.3390/molecules14051660.

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