ISSN : 0974 - 7524 Volume 8 Issue 1

Physical CHEMISTRY
An Indian Journal

Trade Science Inc.

Full Paper

PCAIJ, 8(1), 2013 [27-32]

Improving the mechanical and thermal properties of organic compounds by using simplex method analysis

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ABSTRACT

This paper presents an improvement of organic compounds properties, two cases was analyzed; firstly, the effects of pressure on organic chains. Secondly, the effect of rotating of organic compounds on melting and boiling points. Linear programming and operations research techniques are used here to study such effects. Both tensile strength and elasticity will be improved here by choosing the right pressure applied during the construction of the organic compounds. It is found that the pressure applied during the formation of organic compounds has a significant effect on properties of such compounds, melting and boiling points will be improved here by making some rotation in the bonds between central atom and sub (outer) atoms in the organic compounds under some constraints. The compounds for which these calculations have been made include carbon disulfide, branched thiols, cyclic thiols, aromatic thiols, *n*-alkyl sulfides, branched sulfides, cyclic sulphides (including long-chain *n*-alkylthiolanes and *n*-alkylthianes), aromatic sulfides, *n*-alkyl disulfides, alkylthiophenes, methylated benzothiophenes and dibenzothiophenes,

KEYWORDS

Organic compounds;
Pressure;
Chemical chains;
Organic compounds properties;
Linear programming.

INTRODUCTION

Properties of organic compounds depend on many conditions during the formation, one of such conditions is working pressure, boiling point and melting point, if the pressure is decreased or increased this will give the organic compound new properties or change in expected properties, in this study the tensile strength and elasticity of some given organic compound are studied using operations research methods by constructing a linear program describing the problem and then solving it using simplex method[1].

The challenge behind manufacturing and producing most complex organic compound is to control the pressure other physical properties, in order to avoid any undesired products and achieve high yield of desired material with several mechanical properties. This can be achieved by studying and improvement the mechanical and thermal properties during producing desired organic compounds. It is worth to mention that representing the properties and operating conditions which introduced in this paper, is considered a creative idea which can be developed and used to control most organic material properties in the future.

If the organic compounds rotated either clock wise or counter clock wise for some rotated angle, this will give the organic compound new properties. Melting and boiling points of organic compounds are very important properties which restrict the usage of the organic compound in some conditions especially at hot conditions of use. All recent studies concern on only one type of organic compound and study some thermal and mechanical properties, that because of the enormous number of organic compound which widely differ from each others, also the isomerization and the resonance behavior of carbon atom in organic compounds will generate a new substance with new properties[2].

RELATED WORK

Yi Li, et. al 2009, studied the oxidation operation of some volatile organic compounds (VOCs): such as ethanol, 1-propanol and 2-propanol) over Ag/Al_2O_3 catalyst under the following two conditions: normal atmospheric pressure and temperature conditions and low temperature and pressure conditions. It is found that VOCs were exposed for partial oxidizations, also Alkene is formed under the low pressure conditions, but aldehyde and acid are formed under the normal atmospheric pressure conditions. It is also noticed that low pressure values conditions are more suitable to notice the active intermediates, such as ethanol, ketene and propenal. The study concluded that the pressure has a significant effect on the oxidation pathway of VOCs over Ag/Al_2O_3 catalyst[3].

Ritesh Sanghvi and Samuel H. Yalkowsky, 2006, developed a semi-empirical model for calculating of the boiling points of organic compounds. In that research the boiling point was calculated as the ratio of the enthalpy of boiling to the entropy of boiling[4].

On January 2003, Jihwan Kim *et al* studied the thermal and mechanical stability of epoxy as an organic material using three different of phosphorous; they studied the flammability of epoxy resins at different conditions during formulation reaction. Also, they were able to give a discussion about the encapsulation behavior of the phosphorous during the polymerization[5].

Nicholas J. Turro, replacing the supramolecular organic photochemistry by soft-matter hosts called micelles and hard-matter hosts like porous-solids are discussed with an emphasis on how non-covalent interactions can be systematically exploited to control the catalytic and magnetic effects on the formation of covalent bonds from photochemically produced pairs of radicals[6].

Steven S., et al. studied the solid-phase state of organic compounds and some measurements which are usually made using solvent extraction or thermal headspace analysis. It is also found that volatile organic compounds extracted from the vinyl flooring particles at room temperature by fluidized bed desorption and by direct thermal desorption at elevated temperatures. Also Volatile organics in the extraction gas from fluidized bed desorption and direct thermal desorption were collected on sorbent tubes and analyzed by gas chromatography/mass spectrometry. Also it is found that seven volatile organic compounds emitted by vinyl flooring were quantified. Differences between fluidized beds desorption and direct thermal desorption results may be explained using free-volume/dual-mobility sorption theory[7].

Richard L. and Gaona X studied the relationship between the operating temperature and pressure during formation of organic materials to improve and enhance the standard molal thermodynamics properties based on Gibbs energy amounts of different organic iodine compounds. 13 crystalline, 29 liquid, and 39 ideal gas specimens are tested where the corresponding properties were calculated as a function of operating temperature and pressure. They concluded that the combination between the Gibbs energies which were calculated from experimental measurements and the reduction oxidation conditions can be used to derive an expression able to describe the thermodynamics properties of organic iodine matters[8]. Their study can be considered as introduction to control, improve and enhance the thermodynamics properties of organic iodine materials.

RESEARCH METHODOLOGY

Most of the combination, decomposition, displacement and other types of organic reactions depend on and controlled by the equilibrium correlations which depend basically on the value of pH, temperature and pressure during formation of organic compounds. In 1969, Stull et al. and Pilcher were able to evaluate the equilibrium state of such reactions. Empirically, they recommended calibrating the temperature and pressure at several values to control quantity and quality of produced organic compounds[9,10].

To find the effect of pressure on the organic chains it is assumed that if a positive pressure is applied or if the pressure is increased during organic compound this will affect the tensile strength of the compound and also elasticity by 5 units since the bonds becomes closer and hence strength of bonds becomes more, while the decreasing of pressure will increase the length of the bonds and so the strength and elasticity of the material becomes less by -5 units. If the maximum allowance pressure is 8 units, and for increasing one strength or elasticity of the organic compounds by one unit it needs 3 units of pressure, and 5 units of pressure is needed to decrease the strength of material by one unit. If the maximum difference between positive pressure and minimum one is 10 unite, the compound will need to specify how much positive and negative pressure required increasing or decreasing the strength or elasticity of the organic chain by 5 units. To solve such problems linear programming using operation research techniques are used here especially simplex method.

Firstly the linear program should be constructed, which consists of the objective function; the constraints and the non-negativity.

Objective function

$$\text{Max } Z = 5X_1 + 5X_2 \quad (1)$$

Subject to

$$3X_1 + 5X_2 \geq 8 \quad (2)$$

$$X_1 - X_2 \geq 10 \quad (3)$$

$$X1, X2 \leq 0 \text{ (Non-negativity)} \quad (4)$$

To solve this program simplex method is used. Firstly the program should be written in canonical form as follows:

$$\text{Max } Z = 5X_1 + 5X_2 \quad (5)$$

Subject to

$$3X_1 + 5X_2 + X_3 = 8 \quad (6)$$

$$X_1 - X_2 + X_4 = 10 \quad (7)$$

Non-negativity

$$X_1, X_2, X_3 \text{ and } X_4 \geq 0 \quad (8)$$

The physical and mechanical properties of organic materials are controlled and improved by controlling and evaluation of the rotation angle of molecular chains of those materials. For example, the reduction of rotational energy from 28.8 kJ / mol to 0.5 kJ / mol will change the spin specific gravity for Ubiquinones Q-1, Q-2, Q-6, from 2.572 to 8.321[11]. It is worth mentioning that the physical properties of organic compounds becomes measuring by the frequency of central and side chains of molecular structure of organic compounds. To improve melting or/and boiling point temperatures of any organic compound some rotation clock wise (X_1) or/ and counter clock wise (X_2) are executed. In this study, to get an increase or may be a decrease in such temperature for some organic compound, it is assumed that rotation clockwise will increase the boiling or melting points by about 3ºC, and counterclockwise about 5ºC. If the maximum allowance rotating angle for both directions is 90º, and for increasing one boiling or melting degree temperature it needs 4º CW, and 6º CCW. The maximum difference between clock wise and counter clockwise should not increase more than 30º. Now it needs to specify the degrees needed CW and/or CCW to make this improvement in boiling and melting point temperatures.

To solve such problems, linear programming using operation research techniques are used especially simplex method. Firstly the linear program should be constructed, which consists of the objective function, the constraints and the non-negativity.

Objective function

$$\text{Max } Z = 3X_1 + 6X_2 \quad (9)$$

Subject to

$$4X_1 + 6X_2 \geq 90 \quad (10)$$

$$X_1 - X_2 \geq 30 \quad (11)$$

Non-negativity

$$X_1, X_2 \leq 0 \quad (12)$$

To solve this program simplex method is used.

Firstly the program should be written in canonical form as follows:

$$\text{Max } Z = 3X_1 - 6X_2 \quad (13)$$

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Subject to

$4X_1 + 6X_2 + X_3 = 90$ (14)

$X_1 - X_2 + X_4 = 30$ (15)

Non-negativity

X_1, X_2, X_3, and $X_4 \geq 0$ (16)

RESULTS AND DISCUSSION

The TABLE 1 gives initial tableau of simplex method can be constructed to get the optimal solution of the problem.

TABLE 1: Initial tableau

Basics	Constants	X_1	X_2	X_3	X_4
X_3	8	3	5	1	0
X_4	10	1	-1	0	1
Z	0	-5	-5	0	0

Now, the principles of the Simplex method can be used to solve the problem. Firstly the pivot is chosen as 5,

Now divide the first row by 5 and then the second tableau becomes as:

TABLE 2 : First iteration

Basics	Constants	X_1	X_2	X_3	X_4
X_2	8/5	3/5	1	1/5	0
X_4	58/5	8/5	0	1/5	1
Z	8	-2	0	1	0

The final solution of the problem becomes as shown in TABLE 3.

TABLE 3 : Final solution

Basics	Constants	X_1	X_2	X_3	X_4
X_2	-26/10	0	1	1/8	3/8
X_1	29/4	1	0	1/8	5/8
Z	45/2	0	0	5/4	10/8

The optimal solution is: X_1=29/4 pressure units and X_2=-26/10 pressure unit. i.e. to get an improve in the properties of the organic compound the pressure that should be applied is either 7.25 units of pressure increase or 2.6 pressure units decrease.

It can be noticed that the pressure has a significant role in changing organic compounds properties by improving the properties or may not. But if the ranges of pressure calculated by simplex method are applied at the same assumed conditions the properties will be improved.

The first tableau of simplex method can be constructed to get the optimal solution of the problem.

TABLE 4 : Initial tableau

Basics	Constants	X_1	X_2	X_3	X_4
X_3	90	4	6	1	0
X_4	30	1	-1	0	1
Z	0	-3	-6	0	0

Now, the principles of simplex method are used to solve the problem. Firstly the pivot is chosen as 6, now divide the first row by 6 and then the second table becomes as:

TABLE 5 : First iteration

Basics	Constants	X_1	X_2	X_3	X_4
X_2	15	2/3	1	1/6	0
X_4	45	5/3	0	1/6	1
Z	15	-3/2	6	1	0

The final solution of the problem becomes

TABLE 6 : Final solution

Basics	Constants	X_1	X_2	X_3	X_4
X_2	-3	0	1	1/10	2/5
X_1	27	1	0	1/10	3/5
Z	55.5	0	0	23/20	9/10

So, from the last table

X1=27°, and X2=-3°. i.e. to get an improve in the properties of the organic compound it should be rotated by 27° clockwise and 3° counter clockwise.

Based on the mathematical model which is introduced in this study, the relationship between the different physical properties and the angle of rotation for organic compounds can be graphed as shown in Figure 1. as shown in Figure 1, some physical properties of organic matters are represented as a function of rotational angle for molecular chain. It was noted that the properties proportional linearly with rotational angle for interval between [0°,45°], as the angle of rotation increases more than 45°, the value of all studied properties show disturbance and noise behavior, which means that the material properties cannot be controlled or accurately determined for this interval. It is worth mentioning that dimensionless and scaling techniques were used to represent the actual values of different physical properties of organic compounds.

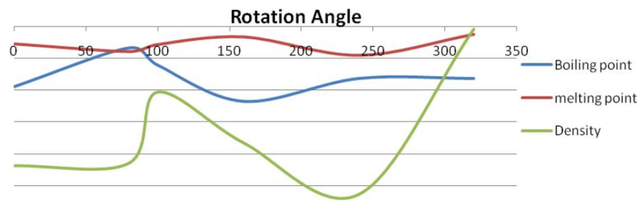

Figure 1 : The relationship between rotational angle of organic chains and different properties; boiling point, melting point and density[11]

According to thermodynamic equations of state for ideal and non-ideal organic gases, the operation pressure in gas media is proportional to the working temperature, so the results are reached in this study can be compared with other researches which studied the physical properties of organic compounds as a function the operation temperature instead of operation pressure, with taken into account that the enthalpy is strong function in temperature[12]. According to Helgeson et al, There is a relationship between thermodynamic properties of organic compound and the applied pressure during formation of such compounds, the study did not mention the reason behind this phenomenon. The model was introduced in this paper discussed the reason of properties variation of organic compounds which is the rotation of functional group in the compound[13].

CONCLUSION

The pressure applied during the formation of organic compounds has a significant effect on properties of such compounds, melting and boiling points will be improved here by making some rotation in the bonds between central atom and sub (outer) atoms in the organic compounds under some constraints.

The operation pressure during organic compounds formation is very important, changing such pressure by increasing or decreasing may change such compounds properties or creating new compounds, it is found that under assumed conditions during organic compounds formation the suitable pressure range was from 26/10 decrease to 29/4 increase.

It can be noticed from last results that the rotation of organic compounds may change or improve the organic compounds properties, under the assumed conditions the range of accepted rotation angles was calculated using linear programs and simplex method to be from 3 degrees clockwise to 27 degrees counter clockwise.

It is worth mentioning that there is a relation between the physical properties of organic compounds and the resonance of the same compounds which produces more radicals of same organic materials. Radical anions were prepared under high-vacuum conditions in alkaline ethanol, with presence of reducing agent under a temperature control.

There are many organic compounds and materials can follow the proposed model such as; carbon disulfide, branched thiols, cyclic thiols, aromatic thiols, *n*-alkyl sulfides, branched sulfides, cyclic sulphides (including long-chain *n*-alkylthiolanes and *n*-alkylthianes), aromatic sulfides, *n*-alkyl disulfides, alkylthiophenes, methylated benzothiophenes and dibenzothiophenes.

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