Mathematical Modeling of Biomass (Wood) Gasification

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Abstract

The paper aims to work theoretical study by using three reactions for the wood burning analysis or (Wood Gasification). First, we suggested a general equation with molar balance modified for the burning. Results obtained, we solved multivariable nonlinear equations non-linear equations by means of Newton-Raphson method. Using the computer program Matlab, we calculated the degree of equilibriums heat for the reactions absolute (946°k, 763 °k, and 68 °k). Also, we calculate thermodynamics functions for the reactions (ΔG, ΔH, K) with two ΔH^+ (non- impulsive) and one ΔH^-(impulsive).

النمــذجة الرياضية لتغويز الوقود الحيوي (الخشب)

الخلاصـــــة

يهدف البحث الى اجراء دراسة نظرية باستخدام تفاعلات ثلاثة لتحليل احتراق الوقود الحيوي(الخشب) او (تغويز الخشب), اولا تم اقتراح معادلة عامة للاحتراق و تم اجراء موازنة عادية (موازنة مولية) للاحتراق. النتائج المستحصلة هو الحصول على اربعة معادلات رياضية تضم سبعة مجاهيل, بعدها تم احتساب عدد المولات باستخدام برنامج الماتلاب, حيث تم احتساب درجة حرارة الاتزان لكل تفاعل من التفاعلات الثلاثة باستخدام طريقة نيوتن – رافسون و كانت درجة حرارة الاتزان للتفاعلات الثلاثة التي حصلنا عليها (946 مطلقة , 763 مطلقة و 68 مطلقة). ايضا تم احتساب الدوال الثرموديناميكية (ΔG , ΔH , k) للتفاعلات الثلاثة حيث بينت النتائج ان التفاعل الاول و الثاني غير تلقائي حيث كانت ΔH موجب و التفاعل الثالث تلقائي و كانت ΔH سالب.

KEYWORDS: Biomass, Gasification, wood, Combustion, Matlab program.

Introduction

Gasification is a process used to generate energy that is cleaner and more efficient than traditional combustion processes. Gasification can be convert these materials into combustible gas, mechanical and electrical power and synthetic fuels and chemicals (Babu and Sheth, 2006).

In this process, the materials that contain carbon-based are broke into a high-energy gas by applying high temperatures in a space containing limited oxygen concentation. High temperatures and little amounts of oxygen allow gasification process to significantly reduce the dangerous emissions. In addition, gasification has other advantages, including active use of waste for energy, efficient method of reduction of waste size, detoxification of dangerous materials (Smith et al., 2004).

In spite of its many advantages, gasification process has always been much expensive to gain a more wide-scale adoption. Many attempts by scientists are being made to advance efficient, flexible, and economic gasifiers for a variety of biomass feedstock in order to minimize the syngas pollution level and maximize the energy output (Nilson et al., 2001).

In the present study, first, been proposed general equation with molar balance modified for the wood burning. Results obtained, we solved multivariable nonlinear equations non-linear equations by means of Newton-Raphson method. Using the computer program Mat lab, we calculated the degree of equilibriums heat for the reactions Also; we calculate thermodynamics functions for the reactions (ΔG, ΔH, K).

Theoretical Study

1. Thermodynamic Equilibrium Model:

Thermal or chemical balance evaluation is not depend on gasifier and so is simple for study the effect of fuel and operation parameters. The chemical or thermal balance may not be achieved within the gasifier; the equation gives the designer with a simple prediction of the maximum available product of a desired product. However, it cannot predict the influence of hydrodynamic or geometric factor, like momentum velocity, or design variables, like gasifier depth. Chemical stoichiometry balance is based on the balance constant as described in the following:

1.1 Assumptions

1. It was assumed that all proposed reactions are perfect reactions.
2. It was taken into consideration the effect of humidity inside the wood.
3. It has been neglecting impurities within the wood.
4. It was considered that all the amount of wood to burn completely without waste.

1.2 Biomass composition

Beginning, from the extra analysis of the wood and the mass fractions of the carbon, hydrogen and oxygen, the subsites wood formula $C_nH_aO_b$ can be estimated, n = 1, with below:

$$a = \frac{H}{C} \quad \text{And} \quad b = \frac{O}{C}$$

Where a and b are the mole fractions of (H/C) and (O/C) determined from the extra analysis of the wood.

From the substitution fuel formula, the general shape of wood is $CH_{1.44}\ O_{0.66} = CH_{0.2}\ (0.6H_2O)$, and therefore the specific molecular weight of the biomass about 24 (M_{Biom}=24). For 1 mole of wood is being gasified in w moles of steam and m moles of air, the global gasification reaction is written as follows:

$$CH_{1.44}O_{0.66} + wH_2O + m\,(O_2 + 3.76N_2) \rightarrow n_1H_2 + n_2CO + n_3CO_2 + n_4H_2O + n_5CH_4 + n_6N_2 + n_7C \qquad (1)$$

Where w is the amount of water per mol of biomass, m is the amount of oxygen per mol of biomass, n_1, n_2, n_3, n_4, n_5, n_6 and n_7 are the stoichiometric coefficients of the products (all stoichiometric coefficients in moles). All inputs on the left-hand side of Eq. (1) are defined at 25°C.

The molar quantity of water per mole of biomass (w) can be determined as:

Let, MC= moisture content per mole of biomass (wood)

$$MC = \frac{\text{Mass of water}}{\text{Mass of wet biomass}} \times 100\% = \frac{M_W\,w}{M_{Biom} + M_W\,w} \times 100\%$$

Therefore, w given by:

$$w = \frac{24MC}{18(1 - MC)} \qquad (2)$$

1.3 Mass balance

C: $$1 = n_2 + n_3 + n_5 + n_7 \tag{3a}$$

H: $$1.4 + 2w = 2n_1 + 2n_4 + 4n_5 \tag{3b}$$

O: $$0.6 + w + 2m = n_2 + 2n_3 + n_4 \tag{3c}$$

1.4 Energy balance

The enthalpy equilibrium equation includes the amount of electricity:

$$\begin{aligned} H^o_{f,Biom} + w(H^o_{f,H_2O(l)} + H_{H_2O(vap)}) + E_{Electricity} &= n_2 H^o_{f,CO} + n_3 H^o_{f,CO_2} + n_4 H^o_{f,H_2O(vap)} + n_5 H^o_{f,CH_4} \\ &+ n_7 H^o_{f,C} + \Delta T(n_1 C_{p,H_2} + n_2 C_{p,CO} + n_3 C_{p,CO_2} \\ &+ n_4 C_{p,H_2O} + n_5 C_{p,CH_4} + 3.76 m C_{p,N_2} + n_7 C_{p,C}) \end{aligned} \tag{4}$$

Where the heat of formation are zero for all chemical elements at reference state (298 K, 1 atm) as:

$$H^o_{f,O_2} = H^o_{f,N_2} = H^o_{f,H_2} = 0$$

where $H^o_{f,Biom}$ is the heat of formation of the biomass material, $H^o_{f,H_2O(l)}$ is the heat of formation of liquid water, $H_{H_2O(vap)}$ is the heat of formation of water vapor, $H^o_{f,CO}$, $H^o_{f,CO2}$ and $H^o_{f,CH4}$ are the heats of formation of the gaseous products, $H^o_{f,C}$ is the heat of formation of solid carbon, C_{p,H_2} , $C_{p,CO}$, C_{p,CO_2} , C_{p,H_2O}, C_{p,CH_4} and C_{p,N_2} are the specific heats of the gaseous products and $C_{p,C}$ is the specific heat of the solid carbon (soot) which is function of temperature (=f(T)), T_2 is the gasification temperature (~1173 K) and T_1 is the ambient temperature (298 K), as $\Delta T = T_2 - T_1$. It is also mentioned that the $E_{Electricity}$ value accounts for the energy required for the gasification reaction.

Eqn. (4) can be simplified to:

$$\begin{aligned} dH_{Biom} + w\,dH_{H_2O(l)} + E_{Electricity} &= n_1 dH_{H_2} + n_2 dH_{CO} + n_3 dH_{CO_2} + n_4 dH_{H_2O(vap)} \\ &+ n_5 dH_{CH_4} + 3.76 m\, dH_{N_2} + n_7 dH_C \end{aligned} \tag{5}$$

Where:

dH for any gas = heat of formation + enthalpy change

$dH_{gas} = H^{o}_{f,gas} + \Delta H$; while $dH_{H_2O(l)} = H^{o}_{f,H_2O(l)} + H_{H_2O(vap)}$; and $dH_{Biom} = H^{o}_{f,Biom}$

At constant pressure, the specific heat can be written as:

$$\Delta H = \int_{T_1}^{T_2} C_{p,mh}\,dT = C_{p,mh}\Delta T \tag{6}$$

Where $C_{p,mh}$ is the average specific heat over the temperature change which is given by:

$$\frac{C_{p,mh}}{R} = A + BT_{am} + \frac{C}{3}\left(4T_{am}^{2} - T_1T_2\right) + \frac{D}{T_1T_2} \tag{7}$$

Where T_{am} is the arithmetic mean temperature and given by:

$$T_{am} = \frac{T_1 + T_2}{2}$$

Also, A, B, C and D are the constants for the properties of the gases concerned (the values of the constants are given in Table 1) and R is the universal gas constant (8.314 J/mol.K).

The enthalpy of formation for solid biomass wood in reactant can be determined (De Souza-Santos, 2004) as:

$$H^{o}_{f,Biom} = LHV_{Biom} + \sum_{k=prod} n_k H^{o}_{f,k} \tag{8}$$

$$\sum$$

1.5 Equilibrium reactions

1. $C + H_2O \rightarrow CO + H_2$ (Primary water gas-shift reaction— endothermic)
2. $CH_4 + H_2O \rightarrow CO + 3H_2$ (Methane decomposition—endothermic)
3. $CO + H_2O \rightarrow CO_2 + H_2$ (gas shift—exothermic)

$$K_i=\prod_i (x_i)^{v_i} \left(\frac{p}{P^{\circ}}\right)^{\sum_i v_i} \qquad (9)$$

Where x_i is the mole fraction of the species i in the ideal gas mixture $x_i = \frac{n_i}{n_{total}}$, $n_{total} = \sum_1^7 n_i$, v is stoichiometric number (positive value for products and negative value for reactants), P° is standard pressure, 1 atm, and n_{total} is total mole of producer gas.

-For the primary water gas shift reaction

$$K_1= \frac{[CO_2].[H_2]}{[H_2O]} \quad \text{or} \quad K_1 = \frac{x_1.x_2}{x_4} \qquad (10\ a)$$

-For the methane decomposition

$$K_2 = \frac{[CO].[H_2]^3}{[CH_4].[H_2O]} \quad \text{or} \quad K_2 = \frac{{x_1}^3.x_2}{x_4.x_5} \qquad (10\ b)$$

-For the water gas shift reaction

$$K_3 = \frac{[CO_2][H_2]}{[CO].[H_2O]} \quad \text{or} \quad K_3 = \frac{x_1.x_3}{x_2.x_4} \qquad (10\ c)$$

The equilibrium constant is a function of temperature only as follow:

$$\ln K = -\frac{\Delta G^{\circ}}{RT} \qquad (11)$$

$$\frac{d\ln K}{dT} = \frac{\Delta H^{\circ}}{RT^2} \qquad (12)$$

$$\ln K = \int \frac{\Delta H^{\circ}}{RT^2} dT + I \qquad (13)$$

Where I is the constant of integration, ΔH° is given in the following equation:

$$\frac{\Delta H^{\circ}}{R} = \frac{J}{R} + (\Delta A)T + \frac{\Delta B}{2}T^2 + \frac{\Delta C}{3}T^3 - \frac{\Delta D}{T} \qquad (14)$$

$$\ln K = \frac{-J}{RT} + (\Delta A)\ln T + \frac{\Delta B}{2}T + \frac{\Delta C}{6}T^2 + \frac{\Delta D}{2T^2} + I \qquad (15)$$

$$\Delta G^{\circ} = -J - RT\left[(\Delta A)\ln T + \frac{\Delta B}{2}T + \frac{\Delta C}{6}T^{2} + \frac{\Delta D}{2T^{2}} + I\right] \qquad (16)$$

Where ΔA, ΔB, ΔC *and* ΔD are calculated for each equilibrium reaction as:

$$\Delta A = \sum_{j=prod} A_i - \sum_{j=reac} A_j \qquad (17a)$$

$$\Delta B = \sum_{j=prod} B_i - \sum_{j=reac} B_j \qquad (17b)$$

$$\Delta C = \sum_{j=prod} C_i - \sum_{j=reac} C_j \qquad (17c)$$

$$\Delta D = \sum_{j=prod} D_i - \sum_{j=reac} D_j \qquad (17d)$$

$$\ln K_1 = f(T) \qquad (18a)$$

$$\ln K_2 = f(T) \qquad (18b)$$

$$\ln K_3 = f(T) \qquad (18c)$$

Results and Discussions

Building-up an equation for each reaction, we calculate the constant factor of heat balance and (ΔG, ΔH, K) for each reaction respectively, in order to find out the amount of energy that produces from gasification under heat degree (1500 °k - 273 °k). By using Matlab program (Newton-Raphson method), we find out (n unknowns and *w*) for the main reaction and energy comes out of each reaction as follow:

1. The first reaction is non- impulsive reaction with (ΔH+) reached heat equilibrium degree (946 °k) and this is logical result because all the carbon turns into CO and CO_2 in temperature high to (600 °k) then it changed to (ΔG–) which means the reactions becomes impulsive at equilibrium degree as shown in figure (1) and we observe decreasing the free energy with increasing reaction temperature as shown in figure (2).Also equilibrium constant is increasing after the temperature (1200 °k).
2. The Second reaction is same as first reaction that is non- impulsive reaction with (ΔH+) reached heat equilibrium degree (763 °k), then it changed to (ΔG–) which means the reactions becomes impulsive after equilibrium degree shown in figure (4) and we observe decreasing the free energy with increasing reaction temperature as shown in figure (5).Also equilibrium constant is increasing after the temperature (1250 K) as shown in figure (6).

3. The third reaction is impulsive reaction with (ΔH–) and staying (ΔH–) and this clear for each imposed temperature degree shown in figure (7) where, we note the large gradient for enthalpy through temperature (250 K), and we observe decreasing the free energy with increasing reaction temperature and approximately similar behavior for free energy in first and second reaction and this shown in figure (8).The equilibrium constant is increasing after the temperature (1200 K) and also approximately similar in behavior for equilibrium constant in first and second reaction and this as shown in figure (9).

Conclusions

1. For the moisture clear effect on the wood combustion process, the more the amount of moisture high whenever moles numbers decreasing of burning wood because of the decreasing in carbonate compounds.
2. In case of non- impulsive reactions when the reaction reaches to equilibrium state, the free energy (ΔG) becomes negative value.
3. The relation between free energy (ΔG) and temperature is linear and this clear in figures (2, 5 and 8) and this identify with theoretical relation for (ΔG) and temperature.

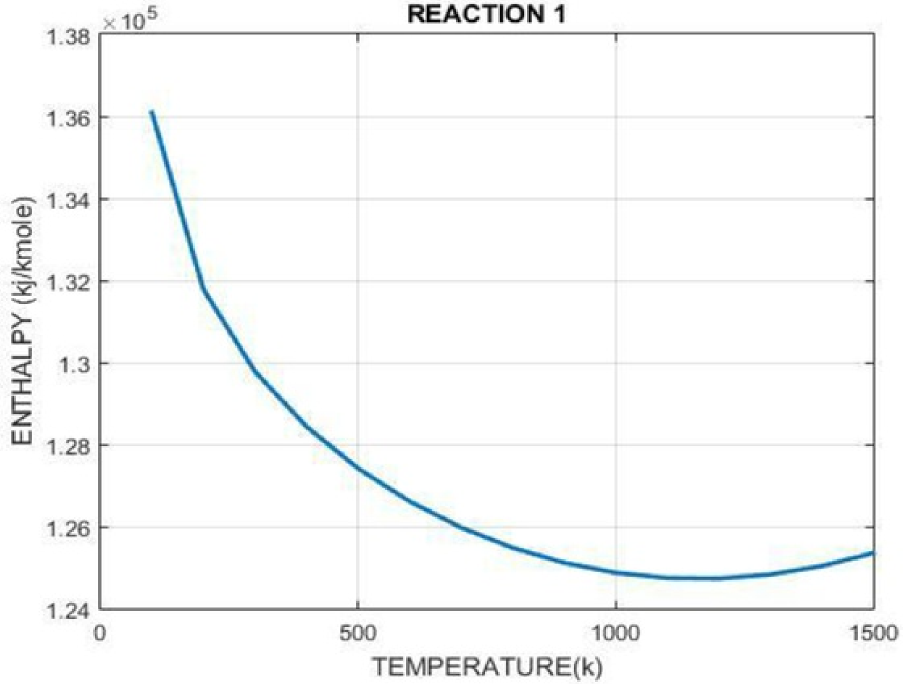

Fig.1 The relation between enthalpy against temperature of R 1

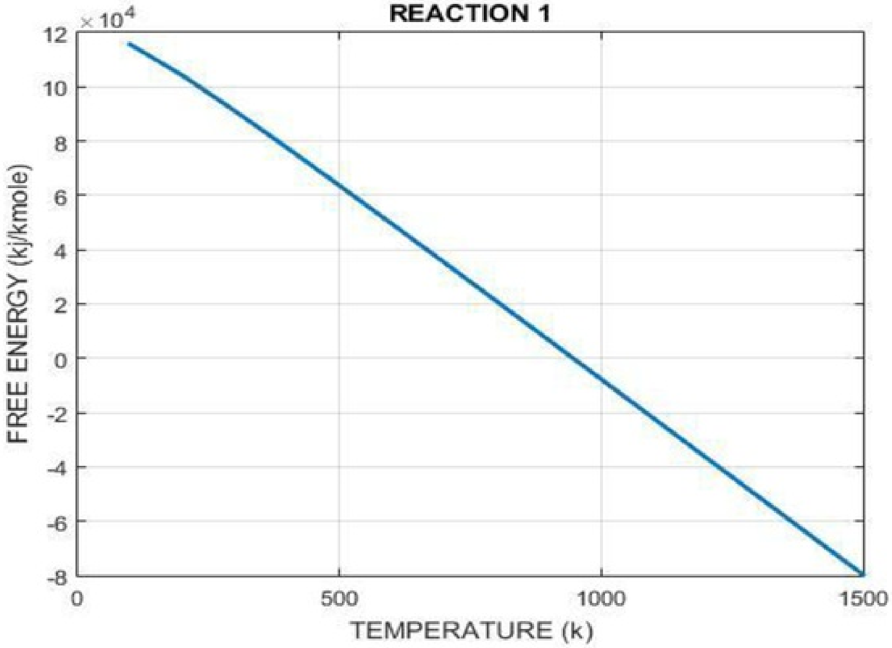

Fig.2 The relation between free energy against temperature Of R 1

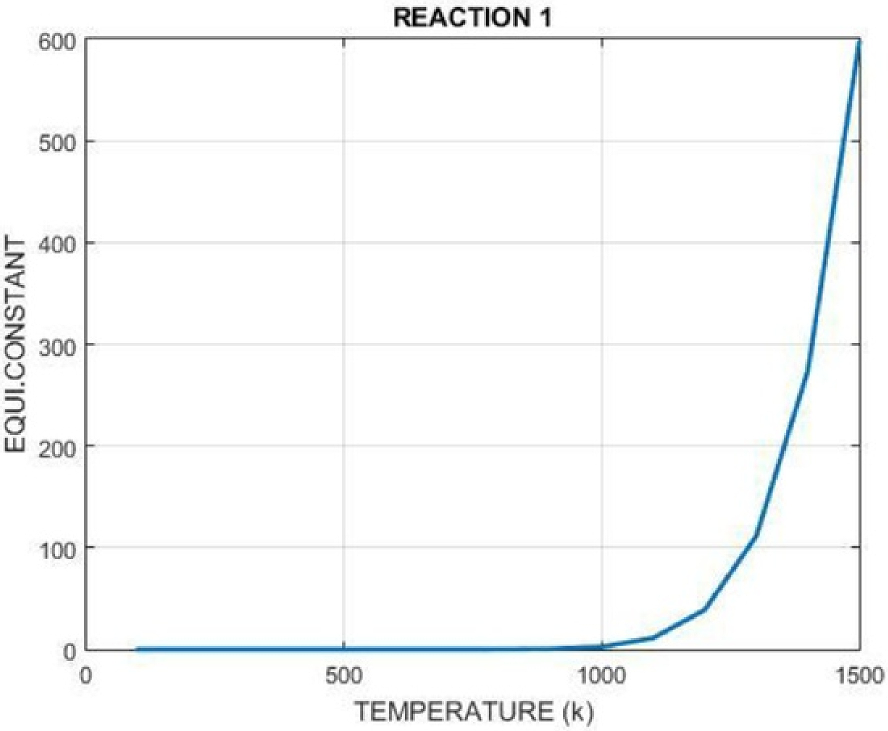

Fig.3 The relation between equilibrium constant against temperature of R 1

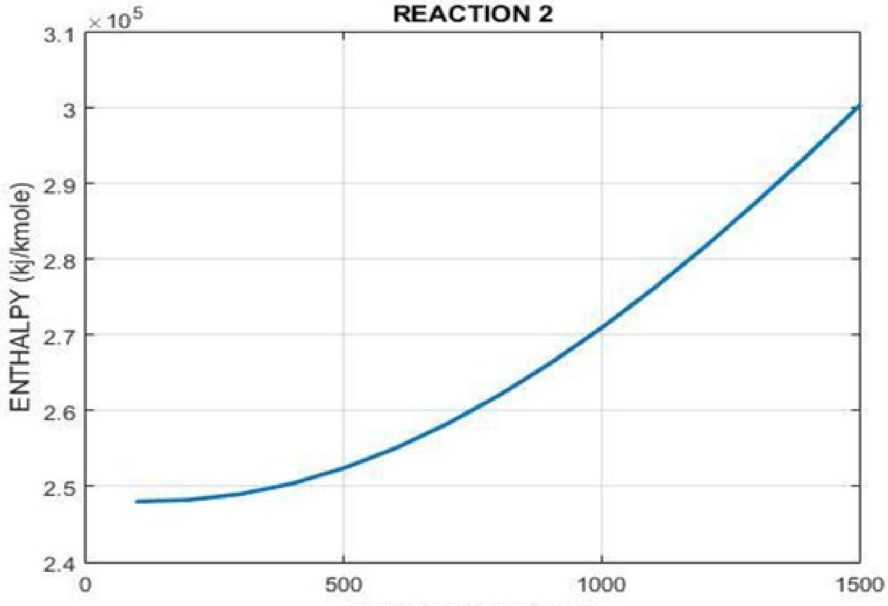

Figure.4 The relation between enthalpy versus temperature of R 2

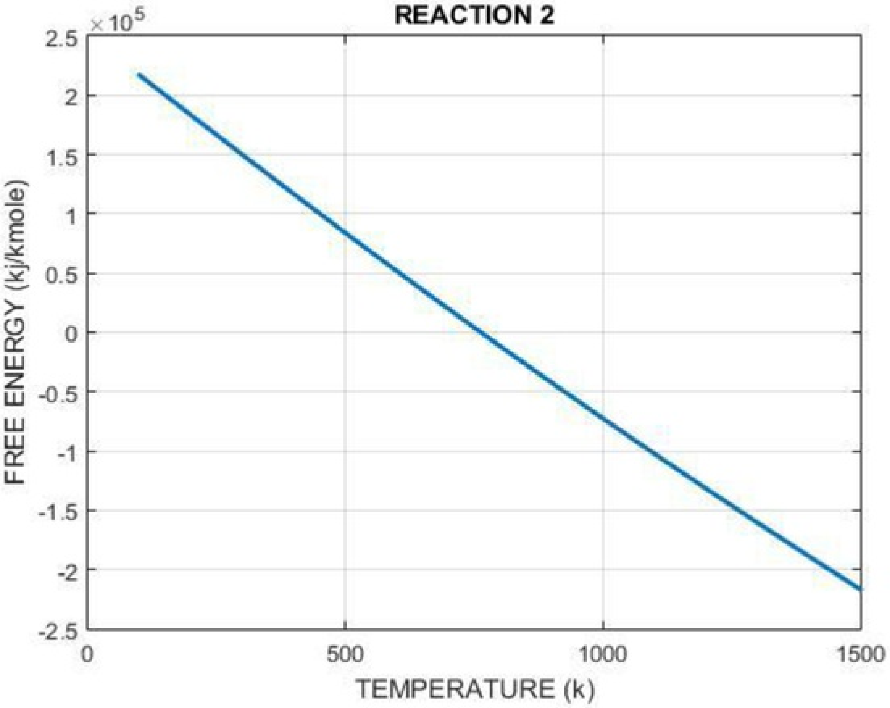

Fig.5 The relation between free energy with temperature of R 2

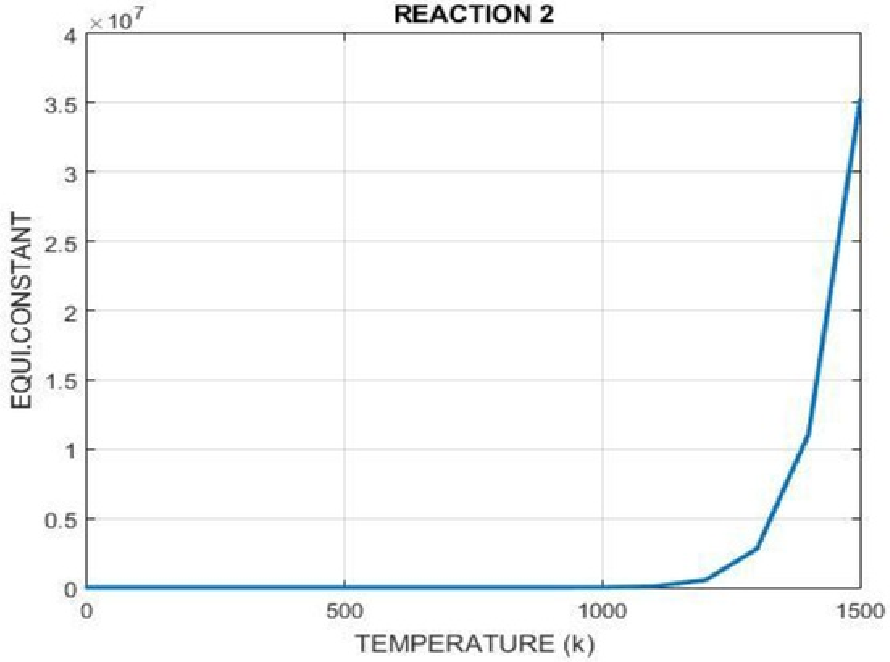

Fig.6 The relation between equilibrium constant versus temperature for reaction 2

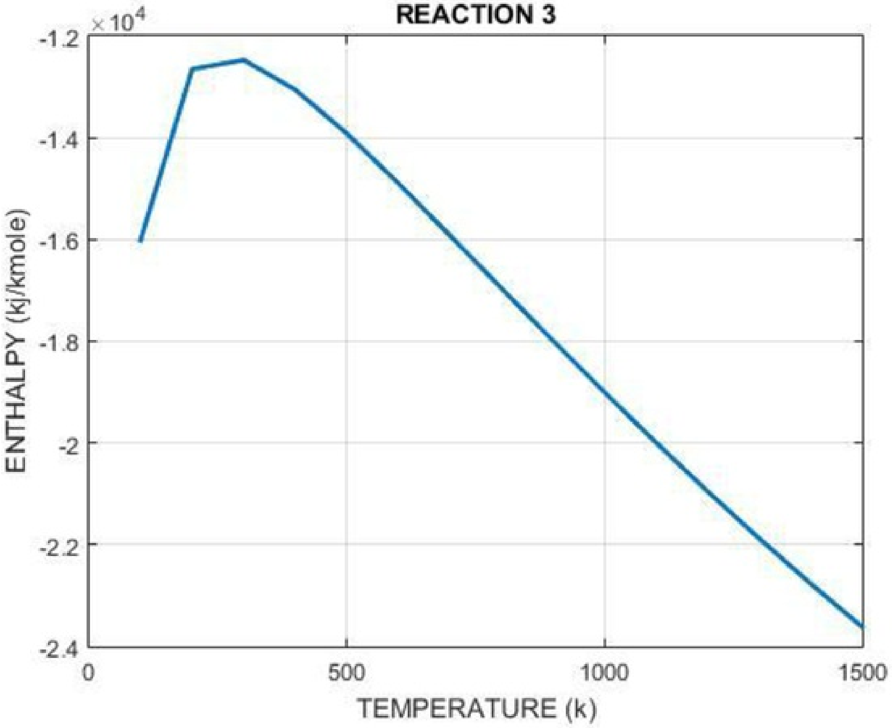

Fig.7 The relation between Enthalpy versus temperature of R3

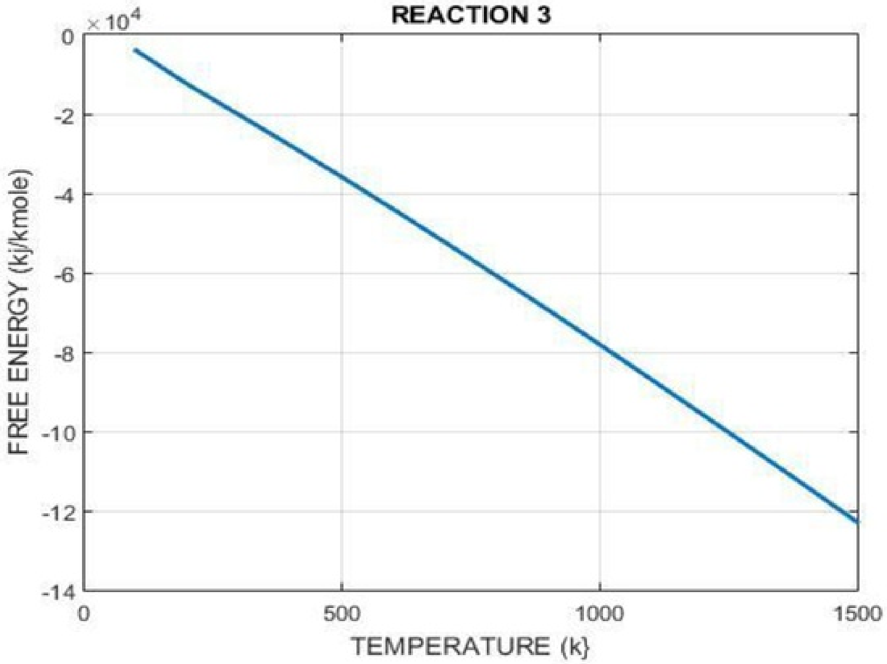

Fig.8 relation between energy versus temperature of R 3

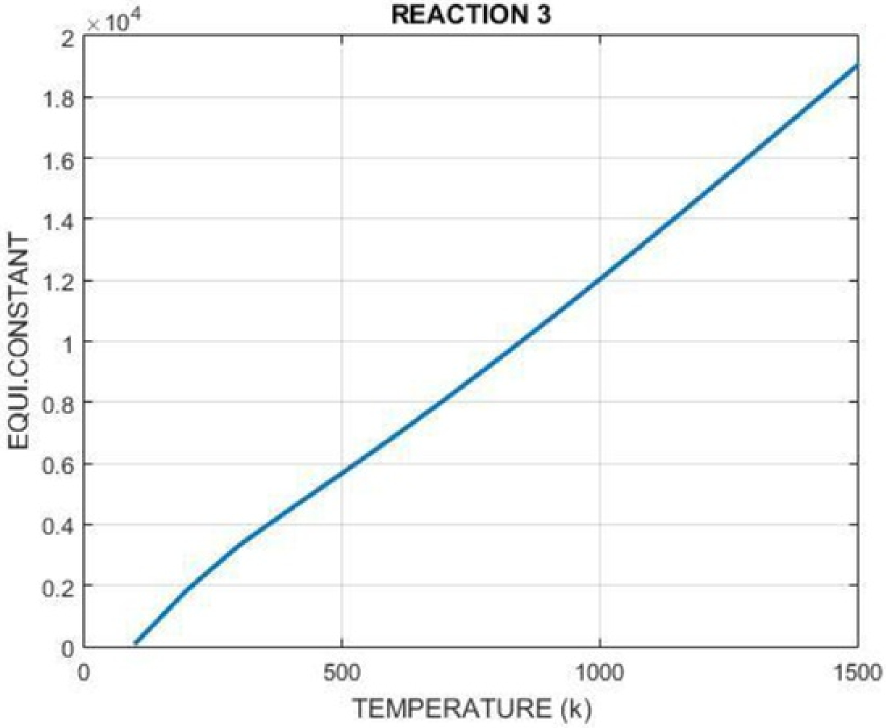

Figure.9 relation between equilibrium constant versus temperature for reaction 3

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