

# Chemical and Combustion Analysis of IRAN Natural Gas with Emission Level

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## Abstract

Natural Gas resources in Iran are located in wide range of area. We divided Natural Gas resources in Iran into 3 categories according to the zone of extraction. The quality of Natural Gas in each of these zones differs from each other. It's better to know which zone of our country has the most appropriate of Natural Gas in quality for Internal Combustion Engines and other zones with less quality for domestic uses and export. Also it's useful to know the combustion characteristics of Natural Gas from each zone of our country and rate of its air pollution in Internal Combustion Engines at different conditions. In this paper, the Natural Gases of Iran are classified upon their chemical properties and heat rate and air pollution level in Internal Combustion Engines with the aid of governing equation and computer simulation from reference (8). We obtained Mean Octant Number and heating value per unit volume of Natural Gas extracted in each zone. Next we calculated heating value of Natural Gas per unit mass in each zone. It is found that the quality of Natural Gas from Northern and East-Northern zone of our country (called zone 3) has advantages for application in Internal Combustion Engines.

## 1. Introduction

Iran has the second rank among the countries of the world which has Natural Gas resources. Chemical characteristics of Natural Gas resources in Iran differs from each other. The Natural Gas in Iran are used for domestic applications and in Internal Combustion Engines. Due to the increasing of population and number of cars in Iran, shortage of liquid fuel, and increasing the air pollution level, the Natural Gas has been used as an alternative fuel for Internal Combustion Engines.

### 2-1. Natural Gas and its quality in Iran

Table (1) shows the calculated calorific values for various types of gasses {8}. The toxic gasses of burning CNG approximately equals to 10% of burning gasoline in Engines, CO is about 20 to 80 percent less. Because the ratio of hydrogen to carbon in methane is high, production rate of CO<sub>2</sub> is less than other fuels.

Calorific value of compounds forming Natural Gas

	Calorific Value (MJ/M <sup>3</sup> )	Calorific Value (MJ/Kg)
Methane	32.79	50.14
Ethane	58.39	47.62
Propane	83.54	46.45
Butane	108.2	45.66
Pentane	133.4	45.34

Table (1)

Considering plentiful resources of natural gas in Iran, conformation of gas is related to location of its extraction. For this purpose, 3 kinds of analyses that are named *Composition 1*, *Composition 2* and *Composition 3* were compared with 100% methane gas, that are respectively gases extracted from the center, the southern and west southern and the northern and finally the east northern zone of Iran {8}. Considering Motor Octant Number (MON) for molar fraction of components in gas in relation (1) and from research done, the relation of critical compression for 3 analyses are given in table (3)

$$MON = (137.78 * X_{methane}) + (29.948 * X_{Ethane}) + (-18.193 * X_{Propane}) + (-167.02 * X_{Butane}) + (181.233 * X_{CO_2}) + (26.994 * X_{N_2})$$

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Percentage of compounds' amplitude of Natural gases in different zones

Northern and East-Northern Zone(3)	Southern and West-Southern Zone(2)	Central Zone(1)	
96.77	84.81	87.81	$CH_4$
1.443	9.5	4.09	$C_2H_6$
0.455	3.61	1.25	$C_3H_8$
0.099	1.03	0.26	$I - C_4H_{10}$
0.174	0.	0.25	$N - C_4H_{10}$
0.72	0.18	0.15	$I - C_5H_{12}$
0.06	0.	0.09	$N - C_5H_{12}$
0.282	0.	0.12	$C_6H_{14}$
0.047	0.37	0.0	$CO_2$
0.598	0.5	5.79	$N_2$

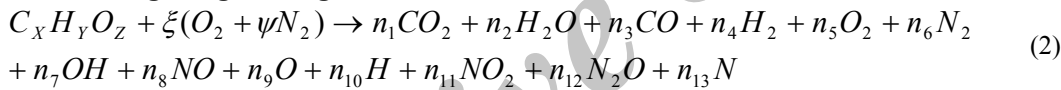
Table (2)

Some characteristics of Natural Gases in different zones

	Zone(1)	Zone(2)	Zone(3)
(MON)			
Motor Octant Number	123	118	133
Critical Compression Ratio	<12.6	<12.4	<13
Calorific Value $MJ / M^3$	33.4	37.7	33.9

Table (3)

### 2-3. Modeling and governing relations



Chemical formula for burning of Natural Gas is replaced with method of calculating multi-componential fuels in equation (2) that for analysis of gases in each three zones are:

Brief presentation of chemical combination of Natural Gas in different zones

Zone(1)	Zone(2)	Zone(3)
$C_{1.037} H_{4.375} O_0 N_{0.115}$	$C_{1.2} H_{4.375} O_{0.007} N_{0.01}$	$C_{1.045} H_{4.76} O_{0.0009} N_{0.012}$

Table (4)

From table(5), we conclude that it's better for us to consume natural gas in third zone of our country for using internal combustion engines and we'd better to extract natural gas in first and second zone of our country for exportation and domestic consumptions, and the reason is that, although calorific value of gas in zone 3 is less than gas in zone 2 in unit volume, considering bulk modulus of elasticity ( $k = -dP/(dV/V)$ ) is low order of magnitude and thus we don't have serious volume restrictions to store natural gas, we must prefer heat value of natural gas per unit mass rather than it's heat value per unit volume.

## 3. Chemical Analysis of combustion chamber In CNG-based Internal Combustion Engines

### 3-1. Terms and Equations governing

In this chapter, we introduce energy equations, chemical equations, chemical equilibrium equations, methods of solving nonlinear equations, experimental relations for fuel injection in cylinder, experimental relations for time and ignition delay and heat transfer.

### 3-2. Energy Equation:

In diesel engines, we can consider gasses in the cylinder as one open system and till intake and exhaust valves are closed, flow of mass is from boundary of the system is only allowed by fuel injection and outgo from the gaps. Neglecting mass flows from the gaps, we can write energy equation for the system as follows:

$$\frac{dQ}{dT} - P \frac{dV}{d\theta} + \dot{m}_f \frac{dt}{d\theta} h_f = \frac{dU}{d\theta}$$

In this equation,  $\frac{dQ}{d\theta}$  is heat flow rate transferred from the system,  $P(\frac{dV}{d\theta})$  is work rate done by the

system by movement of boundary of the system,  $\dot{m}_f$  and  $h_f$  are respectively mass flow rate and enthalpy of fuel injected in the cylinder,  $U$  is internal energy of gases inside the cylinder and  $\theta$  is angle of the crankshaft {4} & {7}. We can use this equation for all strokes except exhaust and induction stroke.

Energy equation for induction stroke is as follows:

$$\frac{dQ}{d\theta} = \frac{dU}{d\theta} + P \frac{dV}{d\theta} - \frac{dH_i}{d\theta} \quad (1)$$

And so energy equation for exhaust stroke is:

$$\frac{dQ}{d\theta} = \frac{dU}{d\theta} + P \frac{dV}{d\theta} + \frac{dH_e}{d\theta} \quad (2)$$

In equations 1 and 2,  $H_i$  and  $H_e$  are respectively enthalpy of inducing and exhausting gases.

### 3-3. Heat release analysis

If we consider  $U$  and  $h_f$  as perceptible internal energy of gasses in the cylinder ( $U_s$ ), then  $\frac{dQ}{d\theta}$  equals the difference between chemical energy released resulted by burning fuel and heat transferred from cylinder enclosure. So we can write equation as follows:

$$\frac{dQ_n}{d\theta} = \frac{dQ_{ch}}{d\theta} - \frac{dQ_{ht}}{d\theta} = \frac{PdV}{d\theta} + \frac{dU_s}{d\theta} \quad (3)$$

In this equation  $Q_n$  is pure calorification,  $Q_{ch}$  is total calorification in combustion chamber and  $Q_{ht}$  is amount of heat transfer from cylinder enclosure.

Assuming gasses in cylinder as ideal gasses, we can write equation 3 as:

$$\frac{dQ_n}{d\theta} = P \frac{dV}{d\theta} + mc_v \frac{dT}{d\theta} \quad (4)$$

And considering the state equation ( $PV=mRT$ ), we have:

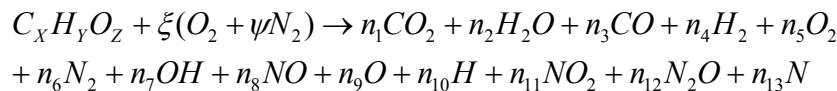
$$\frac{dQ_n}{d\theta} = \frac{\gamma}{\gamma-1} P \frac{dV}{d\theta} + \frac{1}{\gamma-1} V \frac{dP}{d\theta} \quad (5)$$

In the above equation,  $\gamma$  is the ratio of constant pressure specific heat to constant volume specific heat.

$$\left( \gamma = \frac{C_{p,\min}}{C_{v,\min}} \right)$$

### 3-4. Chemical equation of Combustion {3}

Generally, we can consider chemical equation of combustion for a hydrocarbon fuel containing 13 retails in product of combustion as:



In equation 4-3:

X : factor of Carbon in the fuel

Y : factor of hydrogen in the fuel

$n_1$  to  $n_{13}$  : molar coefficients

$\xi$  and  $\psi$  coefficients respectively equals:

$\phi$  :  $\phi$  is equivalence ratio and is ratio of product of ratio of fuel to real air, to product of ratio of fuel to absolute chemical air.

$\left(\frac{F}{A}\right)_a$  is mass ratio of fuel to real air.

$\left(\frac{F}{A}\right)_s$  is mass ratio of fuel to absolute chemical air

$$\xi = \frac{2X + \frac{Y}{2} - Z}{2\phi}$$

$$\psi = 3.773$$

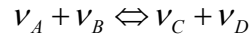
$$\phi = \frac{\left(\frac{F}{A}\right)_a}{\left(\frac{F}{A}\right)_s}$$

### 3-5. Chemical Equilibriums

In sense of GIBS function or free energy, we must say this function is a criterion for equilibrium state sequent of combustion. We introduce this function as follows:

$$G = H - TS$$

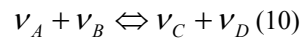
For example we can consider a system initially formed from  $n_A$  mole of substance A and  $n_B$  mole of substance B:



Assuming that the chemical reaction occurred in constant pressure and temperature.

For the extension of Gibbs function to chemical reaction, first we consider a single phase chemical reaction (equal chemical reaction). Imaging of this subject as a gas phase is more advantageous, but the principal of work for all phases is the same.

Consider a reservoir that contains 4 parts A, B, C, D. These retail are possible to be  $CO_2, H_2, CO, H$  in equilibrium in constant compression and temperature. The molar ratios of each retail are shown by  $n_A, n_B, n_C, n_D$ . Moreover the chemical reaction between these four retails are shown as follows:



“v”s are stoichiometry coefficients.

We must emphasis that there is a bright relation between “v”s (stoichiometry coefficients) in the relation 10 while we can change easily the “n”’s for each compound by changing the amount of reservoir component. Now we check the equilibrium provision,  $dG_{P,T}$  for equal chemical reaction. We suppose in the equilibrium, when compression and temperature are constant, the reaction progress tends slightly to the right of the equation.

Thus numbers A and B increase and C & D decrease. Now we show the degree of reaction with  $\epsilon$  and define it as:

$$\begin{aligned} dn_A &= -v_A d\epsilon & (1\_11) & & dn_B &= -v_B d\epsilon & (2\_11) \\ dn_C &= v_C d\epsilon & (3\_11) & & dn_D &= v_D d\epsilon & (4\_11) \end{aligned}$$

The change in the mol number of each fraction in one chemical reaction is obtained by multiplying stoichiometry coefficient with degree of reaction. Also we check the change in Gibbs function for this chemical reaction, that go forward a value of  $d\epsilon$  to the right. For doing this, we must use molar Gibbs fractional function:

$$dG_{T,P} = \bar{G}_C dn_C + \bar{G}_D dn_D + \bar{G}_A dn_A + \bar{G}_B dn_B \quad (12)$$

By replacing  $dn_A$  with  $dn_D$  in the above equation:

$$dG_{P,T} = (v_C \bar{G}_C + v_D \bar{G}_D - v_A \bar{G}_A - v_B \bar{G}_B) d\epsilon \quad (13)$$

Where “G”s are shown as follows:

$$\bar{G}_i = \bar{g}_i^\circ + T \ln a_i \quad (14)$$

By putting “G”s in the equation 13:

$$\begin{aligned} dG_{T,P} &= [v_C(\bar{g}_C^\circ + \bar{R} T \ln a_C) + v_D(\bar{g}_D^\circ + \bar{R} T \ln a_D)] d\epsilon - \\ &[v_A(\bar{g}_A^\circ + \bar{R} T \ln a_A) + v_B(\bar{g}_B^\circ + \bar{R} T \ln a_B)] d\epsilon \quad (15) \end{aligned}$$

Now express  $\Delta G^\circ$  as follow:

$$\Delta G^\circ = \nu_C \bar{g}_C^\circ + \nu_D \bar{g}_D^\circ - \nu_A \bar{g}_A^\circ - \nu_B \bar{g}_B^\circ \quad (16)$$

Equation (16) shows that if the chemical reaction, that contains stoichiometry values for each fraction, completely perform from left to the right of the equation, thus  $\Delta G^\circ$  is changing in Gibbs function. This equation shows that A and B at first are separated in temperature T and standard compression.  $\Delta G^\circ$  is only function of temperature.

By rearranging equation (15):

$$dG_{T,P} = \{\Delta G^\circ + \bar{R} T \ln[a_C^{\nu_C} a_D^{\nu_D} / a_A^{\nu_A} a_B^{\nu_B}]\} d\xi \quad (17)$$

In equilibrium  $dG_{T,P}$  is equal to zero, thus, because  $d\xi$  can take any value, we have:

$$\ln[a_C^{\nu_C} a_D^{\nu_D} / (a_A^{\nu_A} a_B^{\nu_B})] = -\Delta G^\circ / (\bar{R} T) \quad (18)$$

For simplicity:

$$\ln K = -\Delta G^\circ / (\bar{R} T) \quad (19)$$

Or:

$$K = a_C^{\nu_C} a_D^{\nu_D} / (a_A^{\nu_A} a_B^{\nu_B}) \quad (20)$$

### 3-6. Heat of Combustion

Fuel having Hydrogen and Carbon as their main constituents have a heating value intermediate between the heating value of Hydrogen (28600 Kcal/Kg) and that of Carbon (8050 Kcal/Kg) depending on the Hydrogen Carbon ratio of the fuel {5}.

Therefore, the approximate heating value of a hydrocarbon may be expressed theoretically in terms of the percentage by weight of Hydrogen and Carbon or the Hydrogen Carbon ratio. Let C and H be the weight of Carbon and Hydrogen in Kg of fuel.

$$Q_c = [(\% \text{ of } H_2 * 28600) + (\% \text{ of } C * 8050)] / 100$$

$$= \frac{\frac{100}{\frac{C}{H} + 1} * 28600 + \frac{(C/H) * 100}{(C/H) + 1} * 8050}{100} = \frac{28600}{\frac{1}{h} + 1} + \frac{8050}{h}$$

Where h is hydrogen carbon ratio in the fuel (approximately 0.178 for internal combustion petroleum based fuel.) Only approximate heat value of fuel can be obtained by this method. Approximating heating value of natural gasses in Iran:

In zone 1 of our country, consider the formula obtained, we have :

$$C_{1.037} H_{3.954} O_0 N_{0.115} \quad Q_c = (28600 + 8050/h) / (1/h + 1)$$

$$Q_c = 24330.2444 \cong 24330 \text{ (kcal / kg)}$$

h=hydrogen carbon ratio=3.954/1.037

Similarly, in zone 2 of our country, we have :

$$C_{1.2} H_{4.375} O_{.0007} N_{0.01} \quad Q_c = (28600 + 8050/h) / (1/h + 1)$$

$$Q_c = 24176.68161 \cong 24180 \text{ (kcal / kg)}$$

h=hydrogen carbon ratio=4.375/1.2

And finally, in zone 3 of our country, we have :

$$C_{1.045} H_{4.76} O_{.0009} N_{0.012}$$

$$Q_c = (28600 + 8050/h) / (1/h + 1)$$

$$Q_c = 24900.64599 \cong 24900 \text{ (kcal / kg)}$$

h=hydrogen carbon ratio=4.76/1.045

Generally, when two elements, say carbon and hydrogen, unite to form a compound, heat is evolved. The reverse process of splitting up of the compound into its elements requires the expenditure of the same amount of heat.

Therefore, the actual heat of combustion of a fuel, available as a chemical compound, will be less than the value obtained by this method by an amount equal to the expenditure of heat to split up the compound into its constituent.

Now, we introduce the total approximate heating value of natural gas in each zone of our country ( $Q_T$ )

$$Q_T = (\text{weight of hydrogen and carbon} / \text{total weight of gas}) \times Q_C$$

And from Iupac table of elements (1989), we have:

$$C = 12.01115$$

$$H = 1.00797$$

$$O = 15.9994$$

$$N = 14.0067$$

In zone 1 of our country, we have:

$$Q_C = 24330$$

$$C_{1.037} H_{3.954} O_0 N_{0.115}$$

$$Q_{T(1)} = (1.037 \times 12.01115 + 3.954 \times 1.00797) \times Q_{C(1)} \\ / (1.037 \times 12.01115 + 3.954 \times 1.00797 + 0.115 \times 14.0067) \\ \Rightarrow Q_{T(1)} = 22159.02838 \approx 22160 \text{ (kcal / kg)}$$

Similarly, in zone 2 of our country, we have:

$$Q_C = 24180$$

$$C_{1.2} H_{4.375} O_{0.007} N_{0.01}$$

$$Q_{T(2)} = (1.2 \times 12.01115 + 4.375 \times 1.00797) \times Q_{C(2)} \\ / (1.2 \times 12.01115 + 4.375 \times 1.00797 + 0.007 \times 15.9994 + 0.01 \\ \times 14.0067) \\ \Rightarrow Q_{T(2)} = 23860.48341 \approx 23860 \text{ (kcal / kg)}$$

And finally, in zone 3 of our country, we have:

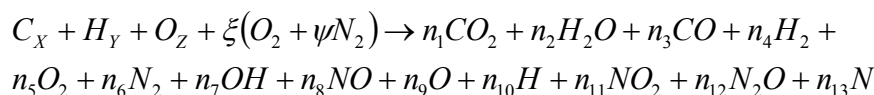
$$C_{1.045} H_{4.76} O_{0.009} N_{0.012}$$

$$Q_C = 24900$$

$$Q_T = (1.045 \times 12.01115 + 4.76 \times 1.00797) \times Q_C \\ / (1.045 \times 12.01115 + 4.76 \times 1.00797 + 0.009 \times 15.9994 \\ + 0.012 \times 14.0067) \\ \Rightarrow Q_T = 24640.83215 \approx 24640 \text{ (kcal / kg)}$$

#### 4. Concept of solving nonlinear equations in order to obtain number in moles of each parts resulted by combustion:

Generally, we define chemical equation of combustion considering 13 molar part resulted by combustion as follows:



For solving our unknowns ( $n_1$  to  $n_{13}$ ) in the above equation, we need 13 equations that 4 equations are obtained by mass balancing of elements carbon, oxygen, hydrogen and nitrogen in. The equation as follows:

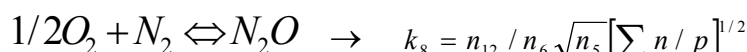
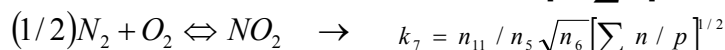
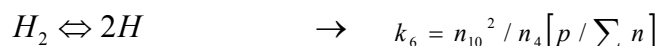
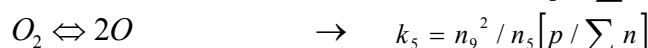
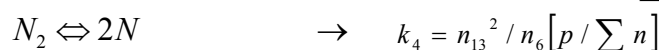
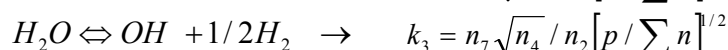
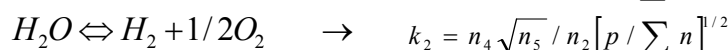
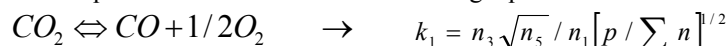
Mass balancing of carbon:  $x = n_1 + n_3$

Mass balancing of nitrogen:  $2\xi\psi = 2n_6 + n_7 + n_8 + n_{11} + 2n_{12} + n_{13}$

Mass balancing of hydrogen:  $y = 2n_2 + 2n_4 + n_7 + n_{10}$

Mass balancing of oxygen:  $2\xi = 2n_1 + n_3 + n_2 + 2n_5 + n_7 + n_8 + n_9 + 2n_{11} + n_{12}$

Other equations are obtained from following equilibrium:



For solving above equations, we can use these methods:

1-newton Raphson method

2-successivesubstitution method

3-combination of method 1,2

#### 4-2. Newton Raphson method

The most usual method for solving nonlinear equations is Newton Raphson method.

Then we consider N equations and N unknowns and write equations in the foregoing forms :

$$f_1 = (x_1, x_2, \dots, x_n) = 0$$

$$f_2 = (x_1, x_2, \dots, x_n) = 0$$

$$f_3 = (x_1, x_2, \dots, x_n) = 0$$

.

.

$$f_n = (x_1, x_2, \dots, x_n) = 0$$

In this method, we must solve partial derivatives of each of the last functions respect to every unknowns as follows :

$$[\partial f_i / \partial x_j] = \begin{bmatrix} \partial f_1 / \partial x_1 & \dots & \partial f_1 / \partial x_2 & \dots & \partial f_1 / \partial x_n \\ \partial f_2 / \partial x_1 & \dots & \partial f_2 / \partial x_2 & \dots & \partial f_2 / \partial x_n \\ \vdots & & \vdots & & \vdots \\ \partial f_n / \partial x_1 & \dots & \partial f_n / \partial x_2 & \dots & \partial f_n / \partial x_n \end{bmatrix}$$

Newton Raphson Method for solving nonlinear equations in additional form is :

$$\sum_{j=1}^n \Delta x_j \frac{\partial f_i}{\partial x_j} + f_i = 0$$

Solving technique for this matrices system is :

$$[\Delta x_j] = -[\frac{\partial f_i}{\partial x_j}]^{-1} [f_i] \quad x_{j,k+1} = x_{j,k} + \Delta x_{j,k}$$

It's obvious that for solving the equations system, we need to solve inverse matrices of the n\*n matrices regarding accession in number of unknowns, time involving for calculations would be long, so we must use another technique. Another restriction of this method in some equations is that answer are not in one range. In such equations, we need to use relaxation in order to avoid divergence factor.

#### 4-3. Successive Substitution

When the equation is in the form that we can write unknowns according to each other.

This method doesn't have a proper convergence when some variables are not zero. Considering equations systems noted when the equivalence ratio (that mentioned previously) is greater Than one or is approximately one, this method has an acceptable convergence.

#### 4-4. Method obtained by combining Newton Raphson method and Successive method

To solve equations systems with this method, some of equations that are in one order are put in Newton Raphson group and some others that are in other orders, are put in successive method group. Regarding above subjects, to solve nonlinear equations system containing 13 molar parts in combustion reaction, we put first 7 equations in Newton Raphson group and consequently we obtain 7 molar parts ratios with matrices inverse method time consumed for calculating decreases because we solve inverse of a 7\*7 matrices rather than inverse of a 13\*13 matrices. After obtaining coefficient of 7 molar parts in reaction equation from this method and replacing them into other 5 equations, we can obtain coefficients of other molar parts from successive substitution method.

We define 1 to 7 functions as follows:

$$\begin{aligned} F_1 &= n_1 + n_3 - x = 0 \\ F_2 &= 2n_2 + 2n_4 + n_7 + n_{10} - y = 0 \\ F_3 &= 2n_1 + n_3 + n_2 + 2n_5 + n_7 + n_8 + n_9 + n_{11} + n_{12} - 2\xi = 0 \\ F_4 &= 2n_6 + n_8 + n_{11} + n_{12} + n_{13} - 2\xi\psi = 0 \\ F_5 &= K_1 n_1 - \sqrt{n_5 p / \sum n n_3} = 0 \\ F_6 &= K_2 n_2 - \sqrt{n_5 p / \sum n n_4} = 0 \\ F_7 &= K_3 n_3 - \sqrt{n_4 p / \sum n n_7} = 0 \end{aligned}$$

Derivatives of functions 1 to 7 accordance to molar parts 1-13 are indicated in form of  $f_{ij} = \partial f_i / \partial n_j$ . indices (i) is related the function number and indices (j) is related to the molar part number.

Permanent coefficients that are related to first 4 equations are:

$$\begin{aligned} f_{11} &= \partial F_1 / \partial n_1 & f_{13} &= \partial F_1 / \partial n_3 & f_{22} &= \partial F_2 / \partial n_2 = 2 & f_{24} &= \partial F_2 / \partial n_4 = 2 & f_{27} &= \partial F_2 / \partial n_7 = 1 \\ f_{210} &= \partial F_2 / \partial n_{10} = 1 & f_{31} &= \partial F_3 / \partial n_1 = 2 & f_{32} &= \partial F_3 / \partial n_2 = 1 & f_{33} &= \partial F_3 / \partial n_3 = 1 & f_{35} &= \partial F_3 / \partial n_5 = 1 \\ f_{37} &= \partial F_3 / \partial n_7 = 2 & f_{38} &= \partial F_3 / \partial n_8 = 1 & f_{39} &= \partial F_3 / \partial n_9 = 1 & f_{311} &= \partial F_3 / \partial n_{11} = 1 & f_{312} &= \partial F_3 / \partial n_{12} = 1 \\ f_{46} &= \partial F_4 / \partial n_6 = 2 & f_{48} &= \partial F_4 / \partial n_8 = 1 & f_{411} &= \partial F_4 / \partial n_{11} = 1 & f_{412} &= \partial F_4 / \partial n_{12} = 1 & f_{413} &= \partial F_4 / \partial n_{13} = 1 \end{aligned}$$

And ratios of equations 5, 6, 7 are as follows:

$$\begin{aligned} f_{51} &= \partial F_5 / \partial n_1 = K_1 & f_{53} &= \partial F_5 / \partial n_3 = -\sqrt{n_5 p / \sum n} \\ f_{55} &= \partial F_5 / \partial n_5 = -1 / 2 \sqrt{n_5 p / \sum n n_3} & f_{62} &= \partial F_6 / \partial n_2 = K_2 & f_{64} &= \partial F_6 / \partial n_4 = -\sqrt{n_5 p / \sum n} \\ f_{65} &= \partial F_6 / \partial n_5 = -1 / 2 \sqrt{p / n_5 \sum n n_4} & f_{72} &= \partial F_7 / \partial n_2 = K_3 \\ f_{74} &= \partial F_7 / \partial n_4 = -1 / 2 \sqrt{p / n_4 \sum n n_7} \\ f_{77} &= \partial F_7 / \partial n_7 = -\sqrt{p n_4 / \sum n n_4} \end{aligned}$$

After obtaining first 7 unknowns with Newton Raphson method and replacing them in low equations, other unknowns are obtained:

$$\begin{aligned} n_8 &= \sqrt{K_9 n_5 n_6} & n_9 &= \sqrt{K_5 n_5 \sum n / p} & n_{10} &= \sqrt{K_6 n_4 \sum n / p} \\ n_{11} &= K_7 n_5 \sqrt{n_6 p / \sum n} & n_{12} &= K_8 n_6 \sqrt{n_5 p / \sum n} & n_{13} &= \sqrt{K_4 n_6 \sum n / p} \end{aligned}$$

Together with obtaining 13 molar parts in computations in one phase and apply convergence term that exerts as follows:

$$\Delta n = \sqrt{\sum_{i=1}^{13} (n_{i,k+1} - n_{i,k})^2} \quad \Delta n < \varepsilon$$

In the above equation,  $\Delta n$  is very small and k indicates the iteration number.

## 5. Conclusions:

From the table(5), we conclude that it's better for us to consume natural gas in third zone of our country for using internal combustion engines and we'd better to extract natural gas in first and second zone of our country



for exportation and domestic consumptions, and the reason is that, although calorific value of gas in zone 3 is less than gas in zone 2 in unit volume, considering bulk modulus of elasticity ( $k = -dP/(dV/V)$ ) is low order of magnitude and thus we don't have serious volume restrictions to store natural gas, we must prefer heat value of natural gas per unit mass rather than its heat value per unit volume .

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### References:

- 1.Natural Gas Engineering Handbook ,By: Guo, Boyun; Ghalambor, Ali, 2005, ISBN :978-0-9765113-3-5
- 2.Internal Combustion Engine Fundamentals ,John Benjamin Heywood ,1989 ,978-0071004992
- 3.Internal Combustion Engines: A Detailed Introduction to the Thermodynamics of Spark and Compression Ignition Engines, Their Design and Development ,1979 ,ISBN: 978-0080227184
- 4.Combstion Engine Processes,Liester C. Lichty ,1967
- 5.Internal Combustion Engine (Theory and Practice),S.P SEN 1984
- 6.Combustion ,Heat transfer and Analysis ,international off-highway and power plant congress & Exposition,1986
- 7.Cycle simulation of direct injection Diesel Engines ,Ahmad Shafiei Saabet ,Shiraz University ,Thesis
- 8.The Fourth International Conference on Internal Combustion Engines ,2005 ,Tehran ,Iran
- 9.مدلسازی موتورهای اشتغال جرقه ای با سوخت گاز طبیعی (CNG) و مقایسه عملکرد انواع گاز طبیعی موجود در کشور، جزایری شوشتری (صفحه 154)
- 9.Iupac Table of Elements ,1989

### Tables:

Calorific Values per unit mass obtained by calculations

	$Q_C$ (kcal / kg )	$Q_T$ (kcal / kg )
Zone1	24330	22160
Zone2	24180	23860
Zone3	24900	24640

From the table below ,we can choose appropriate  $\psi$  's and  $\phi$  's upon the temperature and other properties to analyze .

### Thermodynamic properties of air at low density†

$T$ , K	$h$ , kJ/kg	$u$ , kJ/kg	$\Psi$ $\Phi$		$p_r$	$v_r$	$c_p$ $c_v$		$\gamma$
			kJ/(kg·K)				kJ/(kg·K)		
250	409.9	338.1	4.4505	7.6603	38.81	1849.0	1.003	0.715	1.401
275	435.0	356.0	4.5187	7.7559	54.14	1458.0	1.003	0.716	1.401
300	460.1	374.0	4.5811	7.8432	73.39	1173.0	1.004	0.717	1.400
325	485.2	391.9	4.6385	7.9236	97.13	960.6	1.006	0.718	1.400
350	510.4	409.9	4.6919	7.9982	125.9	797.8	1.007	0.720	1.399
375	535.6	427.9	4.7416	8.0678	160.5	670.8	1.010	0.723	1.397
400	560.8	446.0	4.7884	8.1330	201.4	570.0	1.013	0.725	1.396
425	586.2	464.2	4.8324	8.1945	249.6	488.9	1.016	0.729	1.394
450	611.6	482.5	4.8742	8.2527	305.6	422.7	1.020	0.733	1.392
475	637.2	500.8	4.9139	8.3079	370.4	368.1	1.024	0.737	1.390
500	662.8	519.3	4.9518	8.3606	445.0	322.6	1.028	0.741	1.387
525	688.6	537.9	4.9881	8.4109	530.2	284.3	1.033	0.746	1.385
550	714.5	556.6	5.0229	8.4590	627.1	251.8	1.039	0.752	1.382
575	740.5	575.5	5.0565	8.5053	736.8	224.0	1.044	0.757	1.379
600	766.7	594.5	5.0888	8.5499	860.6	200.1	1.050	0.763	1.376
625	793.0	613.6	5.1201	8.5929	999.5	179.5	1.056	0.768	1.374
650	819.5	632.9	5.1503	8.6344	1155.0	161.5	1.061	0.774	1.371
675	846.1	652.3	5.1796	8.6745	1329.0	145.9	1.067	0.780	1.368
700	872.9	671.9	5.2081	8.7135	1521.0	132.1	1.073	0.786	1.365
725	899.8	691.7	5.2358	8.7512	1735.0	119.9	1.079	0.792	1.362
750	926.8	711.5	5.2628	8.7879	1972.0	109.2	1.085	0.798	1.360
775	954.0	731.6	5.2891	8.8236	2233.0	99.63	1.091	0.804	1.357
800	981.4	751.7	5.3147	8.8584	2520.0	91.12	1.097	0.810	1.354
825	1008.9	772.1	5.3397	8.8922	2836.0	83.52	1.103	0.816	1.352
850	1036.5	792.5	5.3641	8.9252	3181.0	76.71	1.108	0.821	1.350
875	1064.3	813.1	5.3880	8.9574	3559.0	70.58	1.114	0.827	1.347
900	1092.2	833.8	5.4114	8.9889	3971.0	65.07	1.119	0.832	1.345
925	1120.2	854.7	5.4342	9.0196	4419.0	60.08	1.124	0.837	1.343
950	1148.4	875.7	5.4566	9.0496	4907.0	55.58	1.129	0.842	1.341
975	1176.7	896.8	5.4786	9.0790	5436.0	51.49	1.134	0.847	1.339
1000	1205.1	918.1	5.5001	9.1078	6009.0	47.77	1.139	0.852	1.337
1025	1233.7	939.4	5.5212	9.1360	6629.0	44.39	1.144	0.856	1.335
1050	1262.3	960.9	5.5419	9.1636	7299.0	41.30	1.148	0.861	1.333
1075	1291.1	982.5	5.5622	9.1907	8020.0	38.48	1.152	0.865	1.332
1100	1319.9	1004.1	5.5821	9.2172	8797.0	35.90	1.157	0.870	1.330
1125	1348.9	1025.9	5.6017	9.2432	9632.0	33.53	1.161	0.874	1.329
1150	1378.0	1047.8	5.6209	9.2688	10529.0	31.35	1.165	0.878	1.327
1175	1407.1	1069.8	5.6399	9.2939	11490.0	29.36	1.168	0.881	1.326
1200	1436.4	1091.9	5.6585	9.3185	12520.0	27.51	1.172	0.885	1.324

(Table obtained from {2}, Heywood's Internal Combustion Engines Book)