Newton GMRES Method Application to the Methane Partial Oxidation Reaction

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ABSTRACT

Methane partial oxidation is one of the manufacturing processes of synthesis gas which can then be used as an environmentally friendly energy sources. To produce an optimal synthesis gas required an appropriate comparison of the reactants by modeling the problem in a mathematical model. The aim of this paper is to determine the ratio of the feed gas (oxygen and methane) which produces synthesis gas in a partial oxidation of methane by using Newton's GMRES method. Other than that, to analyze the possibility of the formation of solid carbon compounds in the reaction. As if it is done directly through a chemical process is costly and time that is large enough. Establishment of mathematical models is done by utilizing the laws and the general assumptions that apply in the chemical equilibrium reaction. Modeling results in the form system of non-linear equations (SNLE) which will facilitate the analysis of the partial oxidation of methane. Settlement is done using a numerical approach to the Newton GMRES method implemented using Matlab program. The optimal ratio of the number of moles of O2 and CH4 obtained with Newton GMRES method with the same result using Newton's method, which is 0.576715395935549. However, number iterations ie 6 <8. So that the process with the use of Newton's GMRES method is faster than Newton's method.

Keywords: Newton GMRES method, SNLE mathematic model, methane partial oxidation reaction, synthetic gas.

1. INTRODUCTION

Gas-To-Liquid (GTL) Technology is one of technologies currently being developed, because of its ability to process natural gas to produce synthetic liquid fuels that are similar to products of petroleum derivatives, even with better quality. Among the examples of GTL technology are the production of liquid petroleum gas, natural gas from the premium, paraffin, diesel, and wax.

Synthesis gas or syngas is the term given to the gas mixture of carbon monoxide (CO) and hydrogen (H_2) which used to synthesize a wide range of substances such as methanol (CH_3OH) and ammonia (NH_3) (Speight (1991)). One of the process of synthesis gas is by partial oxidation of methane. As for methane partial oxidation reactions occurring simultaneously is as follows:

$$CH_4 + \tfrac{1}{2} O_2 \rightleftharpoons CO + 2H_2$$
$$CH_4 + H_2O \rightleftharpoons CO + 3H_2$$
$$H_2 + CO_2 \rightleftharpoons CO + H_2O$$
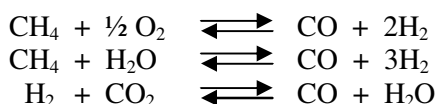
Methane partial oxidation reaction that occurs as a reaction back-reverse (composed of the forward reaction and reverse reaction). When the reaction forward and reverse reactions take place at the same rate there will be a condition of chemical equilibrium. At high temperatures, there may be a reaction formation of solid carbon compounds. In order to create synthesis gas is formed optimally expected solid carbon is formed to a minimum. This is due to the reaction that occurs is that if the equilibrium reaction of solid carbon is formed it will reduce CO formation. Thus, it is necessary to analyze the equilibrium reaction that occurs. When the analysis is done directly by the chemical process will entail large and long enough. It is necessary to be done by other, more profitable, by making a mathematical model of the problem of methane partial oxidation reaction. Subsequently sought a solution with a numerical approach through Newton GMRES method. The aim of this paper is to determine the ratio of the feed gas (oxygen and methane) which produces synthesis gas in a partial oxidation of methane by using Newton's GMRES method. Other than that, to analyze the possibility of the formation of solid carbon compounds in the reaction.

2. METHANE PARTIAL OXIDATION REACTION

Process of methane partial oxidation reaction is a process of combustion of methane with oxygen will produce CO, H_2, H_2O and CO_2 (Brady, (1990)). The main reactions that occurs:

$$CH_4 + O_2 \rightleftharpoons CO + H_2 \tag{1}$$
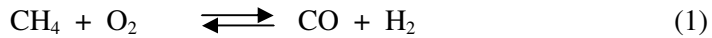
Reaction (1) does not fulfill the law of atomic balance, so that the coefficient of the reaction should be shifted into

$$CH_4 + \tfrac{1}{2} O_2 \rightleftharpoons CO + 2H_2 \tag{2}$$
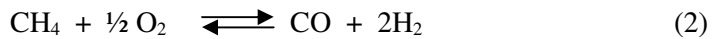
Furthermore, because the reaction (2) is not stable yet to still produce the next reaction which is:

$$CH_4 + H_2O \rightleftharpoons CO + H_2 \tag{3}$$
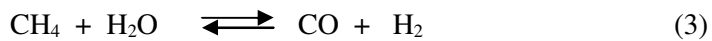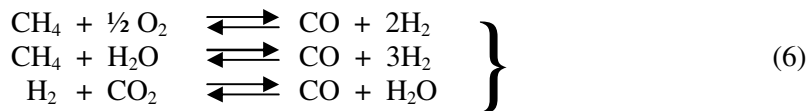
As shown in Reaction (3), that have the same number of hydrogen atoms, so that the coefficient reaction has been changed to:

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \tag{4}$$
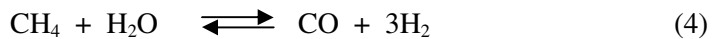
Next, there will be another reaction (5) which has fulfilled the law of atomic balance. The reaction, namely:

$$H_2 + CO_2 \rightleftharpoons CO + H_2O \tag{5}$$
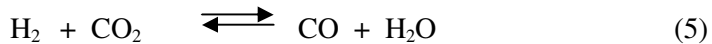
Based on the results of simultaneous reaction of reaction (2), (4), and (5) will be established a system of partial oxidation of methane equilibrium reactions as follows :

$$\left. \begin{array}{l} CH_4 + \tfrac{1}{2} O_2 \rightleftharpoons CO + 2H_2 \\ CH_4 + H_2O \rightleftharpoons CO + 3H_2 \\ H_2 + CO_2 \rightleftharpoons CO + H_2O \end{array} \right\} \tag{6}$$

From the equilibrium reaction (6) obtained an equilibrium reaction mixture, which is generally expressed as follows:

$$wCH_4 + qO_2 \rightleftharpoons rCO + sCO_2 + tH_2O + uH_2 + vCH_4 \tag{7}$$
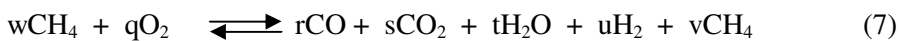
with details :

w = Number of moles of CH_4 in the equilibrium reaction mixture
(as a reactant)

q = Number of moles of O_2 in the equilibrium reaction mixture
(as a reactant)

r = Number of moles of CO in the equilibrium reaction mixture

s = Number of moles of CO_2 in the equilibrium reaction mixture

t = Number of moles of H_2O in the equilibrium reaction mixture

u = Number of moles of H_2 in the equilibrium reaction mixture

v = Number of moles of CH_4 in the equilibrium reaction mixture
(as product)

The equilibrium constant for the reaction at temperatures of 22000F (2), (4) and (5) respectively as follows (Brady (1990), Brice *et al*. (1969)):

$$K_1 = \frac{p_{CO} \cdot (p_{H_2})^2}{p_{CH_4} \cdot (p_{O_2})^{1/2}} = 1,3.e^{11} \tag{8}$$

$$K_2 = \frac{p_{CO} \cdot (p_{H_2})^3}{p_{CH_4} \cdot p_{H_2O}} = 1,7837.e^5 \tag{9}$$

$$K_3 = \frac{p_{CO} \cdot p_{H_2O}}{p_{CO_2} \cdot p_{H_2}} = 2,6058 \tag{10}$$

with p is the magnitude of the partial pressure of 20 atm is used. At a temperature of 2200, each formed of carbon stored in the solid state. Equilibrium constant of reaction (4), namely

$$K_4 = \frac{p_{CO}^2}{a_c p_{CO_2}} = 1329.5$$

with a_c the activity of carbon in the solid state. Dictated by the problem of solid carbon activity is assumed not to be influenced by pressure and the value 1.

Each compound is involved in the process of methane partial oxidation reaction equilibrium has a standard enthalpy values as shown in Table 1. (Roger (1986)).

TABLE 1: Enthalpy of a component at a temperature of 10000F and 22000F

Component	1000°F	2200°F
CH_4	-13492	8427
H_2O	-90546	-78213
CO_2	-154958	-139009
CO	-38528	-28837
H_2	10100	18927
O_2	10690	20831

3. VARIABLE DEFINITION

Based on the reaction equilibrium in the reaction mixture (6) defined some of the following decision variables:

x_1 :　Mole fraction of CO in the equilibrium mixture..

x_2 :　Mole fraction of CO_2 in the equilibrium mixture.

x_3 :　Mole fraction of H_2O in the equilibrium mixture.

x_4 :　Mole fraction of H_2 in the equilibrium mixture.

x_5 :　Mole fraction of CH_4 in the equilibrium mixture.

x_6 :　The number of moles of O_2 per mole of CH_4 in the gaseous reactants.

x_7 :　Number of moles of gas products (CO, CO_2, H_2O, H_2, CH_4) in the equilibrium mixture of CH_4 per mol of the reactant gas.

There are several definitions of other variables to be used in modeling the methane partial oxidation reaction is as follows:

$E_{CH_4}{}^a$: Enthalpy of CH_4 gas at the beginning (the temperature of 1000 ° F)

E_{O_2}　: Enthalpy of O_2 gas at the beginning (the temperature of 1000 ° F)

E_{CO}　: Enthalpy of CO gas at equilibrium (the temperature of 2200 ° F)

E_{CO_2}　: Enthalpy of CO_2 gas at equilibrium (temperature 2200 ° F)

E_{H_2O} : Enthalpy of H_2O gas at equilibrium (the temperature of 2200 ° F)

E_{H_2} : Enthalpy of H_2 gas at equilibrium (the temperature of 2200 ° F)

E_{CH_4} : Enthalpy of CH_4 gas at equilibrium (the temperature of 2200 ° F)

Based on the results of the reaction (7) and defining all the decision variables, then the formula obtained from each of the decision variables as follows:

$$x_1 = \frac{r}{(r + s + t + u + v)} \tag{11}$$

$$x_2 = \frac{s}{(r + s + t + u + v)} \tag{12}$$

$$x_3 = \frac{t}{(r + s + t + u + v)} \tag{13}$$

$$x_4 = \frac{u}{(r + s + t + u + v)} \tag{14}$$

$$x_5 = \frac{v}{(r + s + t + u + v)} \tag{15}$$

$$x_6 = \frac{q}{w} \tag{16}$$

$$x_7 = \frac{(r + s + t + u + v)}{w} \tag{17}$$

4.   ESTABLISHMENT OF MATHEMATICAL MODEL

After defining all the decision variables and consider the rules that apply in the process of methane partial equilibrium reaction, the next step followed by formulating mathematical models. This discussion refers to a previous study conducted by Suryadi *et al.* (2006), which will be explained in the following section.

4.1 Atom Balancing Laws

Defined that the equilibrium number of atoms, ie the number of atoms in the reactants equals the number of atoms around the product (Brady (1990) and Roger (1986)).

Referring to the definition, then from the reaction (7) in the reactant, the CH_4 and O_2 are 1 atom C, 4 H atom and two O atoms (one compound O_2), will be obtained for oxygen that the number of oxygen atoms that enter equal to the number of atoms oxygen in the equilibrium mixture (product).

$$q = \frac{1}{2}r + s + \frac{1}{2}t$$

$$\frac{q}{w} = \frac{\left(\frac{1}{2}r + s + \frac{1}{2}t\right)}{w}$$

$$\frac{q}{w} = \frac{\left(\frac{1}{2}r + s + \frac{1}{2}t\right)}{w} \cdot \frac{(r+s+t+u+v)}{(r+s+t+u+v)} = \frac{\left(\frac{1}{2}r + s + \frac{1}{2}t\right)}{(r+s+t+u+v)} \cdot \frac{(r+s+t+u+v)}{w}$$

$$\frac{q}{w} = \left(\frac{\frac{1}{2}r}{(r+s+t+u+v)} + \frac{s}{(r+s+t+u+v)} + \frac{\frac{1}{2}t}{(r+s+t+u+v)}\right) \cdot \frac{(r+s+t+u+v)}{w}$$

Based on equation (16), (11), (12), and (13) obtained the equation

$$x_6 = (\frac{1}{2}x_1 + x_2 + \frac{1}{2}x_3).x_7$$

$$f_1(x) = \frac{1}{2}x_1 + x_2 + \frac{1}{2}x_3 - \frac{x_6}{x_7} = 0 \tag{18}$$

The same way will be obtained for hydrogen and carbon, namely

$$f_2(x) = x_3 + x_4 + 2x_5 - \frac{2}{x_7} = 0 \tag{19}$$

$$f_3(x) = x_1 + x_2 + x_5 - \frac{1}{x_7} = 0 \tag{20}$$

4.2 The law Energy Proportionality (Enthalpy)

Reaction process of partial oxidation of methane partial done in *diabatically*, that no energy is added or subtracted from the reacting gas. So that the enthalpy (E) of the reactants must be equal to the enthalpy of the

product mixture at equilibrium is reached (Brady (1990) and Roger (1986)). By considering the reaction (7) and variables definition, as well as the enthalpy of the law of proportionality, to be obtained:

$$w.E_{CH_4} + q.E_{O_2} = r.E_{CO} + s.E_{CO_2} + t.E_{H_2O} + u.E_{H_2} + v.E_{CH_4}$$

$$\frac{w.E_{CH_4} + q.E_{O_2}}{w} = \frac{r.E_{CO} + s.E_{CO_2} + t.E_{H_2O} + u.E_{H_2} + v.E_{CH_4}}{w}$$

$$\frac{w.E_{CH_4} + q.E_{O_2}}{w} = \frac{r.E_{CO} + s.E_{CO_2} + t.E_{H_2O} + u.E_{H_2} + v.E_{CH_4}}{w} \cdot \frac{(r+s+t+u+v)}{(r+s+t+u+v)}$$

$$E_{CH_4} + \frac{q.E_{O_2}}{w} = \frac{(r+s+t+u+v)}{w} \cdot \frac{r.E_{CO} + s.E_{CO_2} + t.E_{H_2O} + u.E_{H_2} + v.E_{CH_4}}{(r+s+t+u+v)}$$

$$E_{CH_4} + x_6.E_{O_2} = x_7[x_1.E_{CO} + x_2.E_{CO_2} + x_3.E_{H_2O} + x_4.E_{H_2} + x_5.E_{CH_4}]$$

Substitute the value of the enthalpy of each compound (Table 1), we will obtain:

$$-13492 + 10690x_6 = x_7[-28837x_1 - 139009x_2 - 78213x_3 + 18927x_4 + 8427x_5]$$

$$f_4(x) = -28837x_1 - 139009x_2 - 78213x_3$$
$$+18927x_4 + 8427x_5 + \frac{13492}{x_7} - \frac{10690x_6}{x_7} = 0 \qquad (21)$$

4.3 Limitation of Mol Fraction and Reaction from Equilibrium Relations

The process of partial oxidation of methane partial reactions carried out with the mole fraction range. The assumption is that the number of mole fraction in the equilibrium mixture of a 1 (Brice *et al.* (1969)). Thus, will be obtained a new equation as

$$x_1 + x_2 + x_3 + x_4 + x_5 = 1$$
$$f_5(x) = x_1 + x_2 + x_3 + x_4 + x_5 - 1 = 0 \qquad (22)$$

Reaction that occurs is the reaction equilibrium and oxygen do not react the remaining $(p = 0)$ then equation (8) is not used in the creation of mathematical models, due to the division by 0. Further with respect to the equilibrium constant of equation (9) and defining the decision variables and the partial pressure of $(p = 20)$ atm for each compound is obtained

$$K_2 = \frac{p_{CO} \cdot (p_{H_2})^3}{p_{CH_4} \cdot p_{H_2O}} = \frac{p \cdot x_1 \cdot p^3 \cdot x_4^{\ 3}}{p \cdot x_5 \cdot p \cdot x_3} = 1,7837.e^5$$

$$\frac{p \cdot x_1 \cdot p^3 \cdot x_4^{\ 3}}{p \cdot x_5 \cdot p \cdot x_3} = \frac{p^2 \cdot x_1 \cdot x_4^{\ 3}}{x_5 \cdot x_3} = 1,7837.e^5$$

$$\frac{20^2 \cdot x_1 \cdot x_4^{\ 3}}{x_5 \cdot x_3} = \frac{400 \cdot x_1 \cdot x_4^{\ 3}}{x_5 \cdot x_3} = 1,7837.e^5$$

$$400 \cdot x_1 \cdot x_4^{\ 3} = 1,7837.e^5 \cdot x_5 \cdot x_3$$

$$f_6(x) = 400 \cdot x_1 \cdot x_4^{\ 3} - 1,7837.e^5 \cdot x_5 \cdot x_3 = 0 \tag{23}$$

Whereas for the equilibrium constant of equation (10) with much the same way, the equation is obtained

$$\frac{x_1 x_3}{x_2 x_4} = 2,6058$$
$$f_7(x) = x_1 x_3 - 2,6058 x_2 x_4 = 0 \tag{24}$$

4.4 Result of Mathematics Modelling

Based on the discussion in section 4.1 to 4.3, obtained by mathematical modeling of the problems of methane partial oxidation reaction. The mathematical model is a simple model taking into account the law and the assumption of chemical equilibrium reactions. Because the reaction is taking place simultaneously, then each equation (19), (20), (21), (22), (23), (24) and (25) is obtained by inter-related or otherwise known as a form of mathematical equations system.

Relationship and the nature of the variables in the equation is non linear. Further mathematical model is known as system of non-linear equations (SNLE). The form of mathematical models of problems SNLE methane partial oxidation reaction is:

$$f_1(x) = \frac{1}{2}x_1 + x_2 + \frac{1}{2}x_3 - \frac{x_6}{x_7} = 0$$

$$f_2(x) = x_3 + x_4 + 2x_5 - \frac{2}{x_7} = 0$$

$$f_3(x) = x_1 + x_2 + x_5 - \frac{1}{x_7} = 0$$

$$f_4(x) = -28837x_1 - 139009x_2 - 78213x_3 + 18927x_4 + 8427x_5 + \frac{13492}{x_7} - \frac{10690x_6}{x_7} = 0$$

$$f_5(x) = x_1 + x_2 + x_3 + x_4 + x_5 - 1 = 0$$

$$f_6(x) = 400.x_1.x_4{}^3 - 1,7837.e^5.x_5.x_3 = 0$$

$$f_7(x) = x_1x_3 - 2,6058x_2x_4 = 0$$

with value of $x_i > 0$, $x_i > 0, \forall\ i = 1, 2, ..., 7$.

Based on the form of SNLE it will look for a solution approach (x_i with $i = 1, 2, ..., 7$, in this case primarily the value of x_6) by using Newton's GMRES method.

5.   NEWTON GMRES METHOD

Newton GMRES method is a modification of Newton's method with the newton step was obtained using the GMRES method (Burden *et al.* (1997)). Suppose given a SNLE $F(x) = 0$. Then according to Newton's method to obtain an approximation of the value of x which satisfies the equation $F(x) = 0$, the sought value of the newton step as follows

$$s = -F'(x)^{-1}F(x)$$

$$F'(x)s = -F(x) \tag{25}$$

Thus, if equation (26) fitted to the equation, $Ax = b$, then the relationship is obtained:

a. Matrix A replaced by $F'(x)$
b. Value x replaced by s, with $s_k = x_{k+1} - x_k$
c. Value b replaced by $= -F(x)$

Here is presented a method of Newton GMRES algorithm, named algorithm nsolgm, in solving a problem SNLE $F(x) = 0$ (Burden *et al.* (1997)). nsolgm algorithm requires several input which are the function $F(x)$, previous approximately value, the value of tolerance and a forcing term, which ensures that the error of the approximation solution to a smaller iteration of the previous iteration.

Algoritma nsolgm (x, F, τ, η)

1. $r_c = r_o = \left\|F(x)\right\|_2 \big/ \sqrt{N}$
2. Do while $\left\|F(x)\right\|_2 \big/ \sqrt{N} > \tau_r r_0 + \tau_a$

    (a) Select η
    (b) fdgmres (s, x, F, η)
    (c) $x = x + s$
    (d) Evaluate $F(x)$
    (e) End while

In th step 2(b) of the algorithm is invoked nsolgm to fdgmres procedure, in solving linear problems, which returns the value of the Newton step s to repair the approximation solution of SNLE. Here is presented an algorithm to search for newton step, $s = -F'(x)^{-1} Fx$ is named fdgmres algorithm that uses forward approach approximation difference in the value of $F'(x)$ (Burden *et al.* (1997)).

Algoritma fdgmres $(s, x, F, h, \eta, \text{kmax}, \rho)$

1. $s = 0, r = -F(x), v_1 = r \big/ \left\|r\right\|_2, \; \rho \left\|r\right\|_2, \; \beta = \rho, \; k = 0$
2. While $\rho > \eta \left\|F(x)\right\|_2$ kmax do

(a) $k = k + 1$

(b) $v_{k+1} = D_h F(x : v_k)$

    For $j = 1, ..., k$

    (i) $h_{jk} = v_{k+1}^T v_j$

    (ii) $v_{k+1} = v_{k+1} - h_{jk} v_j$

(c) $h_{k+1,k} = \left\| v_{k+1} \right\|_2$

(d) $v_{k+1} = v_{k+1} / \left\| v_{k+1} \right\|_2$

(e) $e_1 = 1, 0, ..., 0)^T \in R^{k+1}$

    minimize $\left\| \beta e_1 - H_k y^k \right\|_{R^{k+1}}$ to obtain $y^k \in R^k$

(f) $\rho = \left\| \beta e_1 - H_k y^k \right\|_{R^{k+1}}$

(g) End while

3. $s = V_k y^k$

In step 2(b) sought approximation of $F'(x)$ using the *forward difference* approach to the directional derivative is defined as follows (Kelley (1995)):

In example, F is defined in a chromosome of $x \in R^n$ dan $w \in R^n$ and then obtained:

$$D_h F(x : w) = \begin{cases} 0, & w = 0 \\ \left\| w \right\| \ F(x + h \left\| x \right\| (w / \left\| w \right\|)) - F(x), & w, x \neq 0 \\ \left\| w \right\| \dfrac{F(h(w / \left\| w \right\|)) - F(x)}{h}, & x = 0, w \neq 0. \end{cases}$$

In step 2(e) is used to complete the given rotation minimizes the *least square* problem $\left\| \beta e_1 - H_k y^k \right\|_{R^{k+1}}$. In step 3, the calculated amount is expected to improve the *newton step* solution of $F(x) = 0$.

6. RESULT OF NEWTON GMRES METHOD IMPLEMENTATION

Furthermore, the results indicated the implementation of Newton's GMRES method in solving problems of partial oxidation of methane in the SNLE models using Matlab program. Output is obtained depending on each initial value.

Experiments have been performed in 52 cases. Some results of these experiments are presented in Table 3 and the best solution discovered is the case for-51 with a value of [0.3: 0.1: 0.1: 0.6: 0.1: 0.5; 3]. The selection of the best solution based on the number of outer iterations and inner iterations required to obtain an approximation solution of SNLE. With the initial value of the outer iterations are needed as much as 6 iterations and iterations in as many as 37 iterations, the error of 12.278862985274519e-012, and the solution as shown in Table.2

TABLE 2: Best Approximation Solution

Approximation Solution	Error	Outer iteration
x(1) : 0.322870839476541 x(2) : 0.009223543539188 x(3) : 0.046017090960632 x(4) : 0.618171675070824 x(5) : 0.003716850952815 x(6) : 0.576715395935549 x(7) : 2.977863450791146	2.278862985274519e-012	6

Based on the best solution obtained can then be calculated amount of solid carbon formation equilibrium constant $(\overline{K})$ by reaction (4) is

$$\overline{K} = \frac{p^2 co}{a_c p\, co_2} = \frac{(p * x_1)^2}{a_c (p * x_2)} = \frac{400 * (x_1)^2}{1 * 20 * x_2}$$

Other results of the experiments have been conducted (see Table 3) shows that the magnitude of $\overline{K} = 226.042363309468330$. Based on the constant formation of solid carbon at the temperature of the oxidation reaction is $K_4 = 1329.5$, so that $\overline{K} < K_4$. Means there is no tendency that the solid carbon will be formed with the resulting composition in the case to-51.

The experimental results of 52 cases showed that for all feasible solutions, the equilibrium value obtained $\bar{K} < K_4$. Thus proved that there is no tendency of solid carbon is formed for all variable solutions

TABLE 3: SNLE partial solution based on 52 different initial values

Case	Initial Values	Approximation Sollution	Error	$\bar{K}$	$\sum IL$	$\sum ID$
1	0.1 0.5 0.5 0.5 0.5 0.5 0.5	0.322870839476541 0.009223543539188 0.046017090960632 0.618171675070824 0.003716850952815 0.576715395935549 2.977863450791145	1.819003284881415e-012	226.042363309468330	9	55
3	0.3 0.5 0.5 0.5 0.5 0.5 0.5	0.322870839476510 0.009223543539190 0.046017090960642 0.618171675070759 0.003716850952899 0.576715395935431 2.977863450790640	7.047870449025783e-010	226.042363309355490	9	54
9	0.5 0.2 0.5 0.5 0.5 0.5 0.5	0.322870839476540 0.009223543539188 0.046017090960632 0.618171675070823 0.003716850952817 0.576715395935547 2.977863450791138	9.621199937794145e-012	226.042363309466880	9	58
⋮	⋮	⋮	⋮	⋮	⋮	⋮
42	0.5 0.5 0.5 0.5 0.5 0.7 0.5	N/A				
44	0.5 0.5 0.5 0.5 0.5 0.5 0.2	0.322870839476537 0.009223543539188 0.046017090960633 0.618171675070817 0.003716850952824 0.576715395935537 2.977863450791091	1.819003284881415e-012	226.042363309455570	12	71

TABLE 3 (continued): SNLE partial solution based on 52 different initial values

Case	Initial Values	Approximation Sollution	Error	$\bar{K}$	$\sum IL$	$\sum ID$
51	0.3 0.1 0.1 0.6 0.1 0.5 3	0.322870839476541 0.009223543539188 0.046017090960632 0.618171675070824 0.003716850952815 0.576715395935549 2.977863450791146	2.278862985274519e-012	226.042363309468330	6	37
52	0.3 0.2 0.1 0.6 0.2 0.5 0.3	0.322870839476541 0.009223543539188 0.046017090960632 0.618171675070824 0.003716850952815 0.576715395935549 2.977863450791145	1.819044928250029e-012	226.042363309468410	7	41

* $\sum IL$ = *outside iteration number ;* $\sum ID$ = *inner iteration number*

The optimal ratio of the number of moles of O2 and CH4 obtained with Newton GMRES method with the same result using Newton's method, which is 0.576715395935549. However, number iterations ie $6 < 8$. So that the process with the use of Newton's GMRES method is faster than Newton's method.

7. CONCLUSION

The issues of methane partial oxidation reaction equilibrium can be modeled with the form of mathematical modeling. These efforts are by using careful attention to the rules (laws) and the assumption of the methane partial oxidation reaction. SNLE based models will be easy to analyze the process of methane partial oxidation reaction is optimal. Analyses were performed based on the results of the settlement SNLE using Newton GMRES method, namely that the resulting synthesis gas reaction equilibrium and the maximum mole ratio of oxygen (O_2) and mol methane (CH_4) is equal to 0.576715395935549 (value of x_6). In addition, there is no solid carbon formation tendency in the partial oxidation of methane is based on the results of the equilibrium constant value, namely the formation of solid carbon $\bar{K} = 226.042363309468330$ and $K_4 = 1329.5$ ($\bar{K} < K_4$).

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