Study on the effect of lowering steam to carbon ratio in combined reforming of natural gas to the synthesis gas.

By

Lau Swee Leong

Dissertation submitted in partial fulfillment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

July 2003

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CERTIFICATION OF APPROVAL

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Approved by,

……………………………….
(Puan Nurhayati Melon)

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ABSTRACT

The objective of this research is to study the effect of lowering Steam to Carbon ratio in a combine reformer to produce syngas in order to optimize the performance of the combine reformer. A combine reformer in this project refers to the combination of steam methane reformer (SMR) and autothermal partial oxidation reformer (POX). Currently the steam to carbon molar ratio is maintaining at 3:1 ratio in order to prevent carbon deposition on the nickel catalyst active surface. To achieve this, a simulation model of the reformer unit using HYSYS simulation software version 3.01 was develops.

The preliminary stage of this research will focus on literature review of natural gas reforming technology. Then second stage will focus on research for reaction kinetics on the SMR and POX reaction. A simulation model will then be developed to further analyze the reforming process by manipulating the operating condition and S/C ratio. Finally the last stage of the research will focus on optimizing the operation of both reformers.

Based on the simulation result and analysis on various S/C ratio, this project suggest that operating the steam methane reformer using S/C molar ratio of 2:1 instead of 3:1 is favorable to methanol synthesis since carbon monoxide and carbon dioxide molar is increased at S/C ratio of 2:1 and the amount of hydrogen produced is still in excess to cope for the methanol synthesis requirement. However, since there is no physical experiment to determine the actual carbon boundary, there is no strong basis to prove that operating at S/C ratio at 2:1 will curb the carbon deposition problem. A conservative suggestion will be to lower down the S/C ratio to 2.5:1, saving 14 tons per hour of steam and its associated boiler feed water BFW treatment cost while increasing methanol production. A detail experiment to determine the actual carbon boundary is recommended since literature has been reported that optimum S/C ratio between 1.9 and 4.5 for SMR.

ACKNOWLEDEMENTS

The success of writing this dissertation owes its shape and form to the assistance and hard work of many people from the beginning of this final year research until the born of this dissertation. I would like to take this great opportunity to express my deepest gratitude to the following personnel who kindly guided me, giving full support and continuously advise on both technical and non-technical aspect.

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CHAPTER 1
INTRODUCTION

1.1 Background of study

Synthesis gas or more commonly known as syngas is a general term used to describe mixture of hydrogen gas and carbon monoxide gas. These gases are crucially important building block of many more valuable and important petrochemical product such as methanol or [1]ammonia. The source of syngas may come from many types of process and feedstock yielding different composition and syngas ratio. Syngas ratio is defined as molar ratio of hydrogen gas over carbon monoxide gas, H_2/CO, and different process requires different H_2/CO molar ratio [1] listed in table below:

Table 1.1: Syngas ratio requirement for different petrochemical processes.

Ratio	Main use
$1\ H_2$	Refinery hydrotreating and hydrocracking
$3\ H_2: 1\ N_2$	Ammonia Synthesis
$2\ H_2: 1\ CO$	Alkenes (Fisher-Tropsh reaction)
$2\ H_2: 1\ CO$	Methanol, higher alcohol
$1\ H_2: 1\ CO$	Aldehydes (hydroformylation)

Typical syngas converting processes are steam-methane reforming, CO_2 dry reforming, partial oxidation or gasification of coal or petroleum coke, autothermal reforming and water electrolysis [1]. Natural gas usually are the typical feedstock for syngas production, however, other feedstock like liquified petroleum gas, oil, higher hydrocarbon, naptha also can be used to produce syngas [1-3].

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[1] Mixture of N_2 and H_2 for ammonia synthesis also refers as syngas [3].

Steam-methane reforming process is a metal catalyzed reaction described via two stoichiometry reactions.

$$CH_4 + H_20 \Leftrightarrow CO + 3H_2; \Delta H= +206kJmol^{-1} \qquad (1.1.1)$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2; \Delta H = -41kJmol^{-1} \qquad (1.1.2)$$

Natural gas with methane being the major component is mixed with steam and reacts over nickel catalyst in reformer tubes. The reaction heat is supply by radiant heat via combustion of hydrocarbon fuel from the reformer furnace at a typical operation temperature of 600-800°C, and pressure of 30-40 Bar [6-7].

Autothermal reactor on the other hand, is the combination of partial oxidation process and steam reforming process in a single reactor. Pure oxygen is mixed with natural gas with a proper combustion ratio prior inlet of the autothermal reactor, then partial and complete methane oxidation reaction will occur in the combustion zone according to stoichiometry reactions below:

$$CH_4+1/2O_2 \rightarrow CO+2H_2 \qquad \Delta H= -21.8 \text{ kJmol}^{-1} \qquad (1.1.3)$$

$$CH_4+2O2 \rightarrow CO_2+2H_2O \qquad \Delta H= -803 \text{ kjmol}^{-1} \qquad (1.1.4)$$

Notice that both oxidation processes are highly exothermic reaction, thus large amount of heat is liberated during reactions typically around 900 to 1200°C. Taking advantage of this large heat amount, the produced syngas will pass through a catalyst bed at the middle of the reactor to undergo secondary steam reforming process as stated in reaction (1.1.1) and (1.1.2) to further convert any remaining methane reactant. In fact, the term "autothermal" is derived from transfer of exothermic reaction heat to endothermic reaction phenomenon in this reformer [1-2].

Economic evaluation for selection of a syngas process depends upon the required hydrogen to carbon monoxide molar ratio, availability and the cost of hydrocarbon feedstock, availabilty and cost of oxygen and carbon dioxide gas, utilities cost and credit available for excess steam, hydrogen or carbon monoxide gas. Thus, there is an ample opportunity for different combination of syngas conversion process.

The aim of this project is to minimize the S/C ratio to 2:1 from an initial value of 3:1 in a combine reformer to produce syngas for methanol synthesis production. Combine reformer here refers to the combination of steam methane reformer (STM) and autothermal partial oxidation reformer (POX). Rationale of combining autothermal reformer with steam reformer is that steam reforming normally producing excess Hydrogen gas compare to Carbon monoxide with H_2/CO ratio of 6:1, such high ratio of hydrogen gas will yield little production of methanol in the synthesis reactor downstream. Thus integrating autothermal reactor with partial oxidation of the unconverted natural gas from steam reformer will yield more carbon monoxide gas and carbon dioxide gas to give a better proportion of syngas ratio. Ultimately improving the production of methanol product.

1.2 Problem statement

According to the process kinetic model suggested by Rostrup and Nelson [6,7], steam reforming involves the decomposition of hydrocarbon into C, CH_3 and CH_2 fragment on the catalyst metal surface. At the same time, steam molecule also dissociated to hydrogen and oxygen atoms and adsorbed on the surface of the catalyst. Next the free oxygen atom will combine with hydrocarbon fragment to form Carbon Monoxide or Carbon dioxide. Finally, the formed carbon monoxide, carbon dioxide and hydrogen gas will diffuse back to the bulk flow. The proposed kinetic model is elucidates as below:

- $C_nH_m + 2S^+ \rightarrow C_nH_z\text{-}S_2 + \frac{m-z}{2}H_2$ (1.2.1a)
- $C_nH_z\text{-}S_2 + nS^+ \rightarrow C_{n-1}H_{z'}\text{-}S_2 + CH_x\text{-}S_n$ (1.2.1b)
- $CH_x\text{-}S_n + nS \rightarrow CO + \frac{x}{2}H_2 + (n-1)S$ (1.2.1c)
- $H_20 + S \Leftrightarrow O\text{-}S + H_2$ (1.2.1d)
- $H_2 + 2S \Leftrightarrow 2H\text{-}S$ (1.2.1e)

Problem may arises when the carbon removal rate by oxygen atom from steam molecule is lower than the carbon deposition rate. Then successive carbon built up might increase the pressure drop across the catalyst tube.

This problem is made more complicated via coke formation reactions: (1.2.1) Bouduard reaction, (1.2.2) reaction between carbon monoxide and hydrogen, and (1.2.3) methane cracking [2].

$$2CO \Leftrightarrow C + CO_2 \qquad (1.2.2)$$
$$CO + H_2 \Leftrightarrow C + H_2O \qquad (1.2.3)$$
$$CH_4 \Leftrightarrow C + 2H_2 \qquad (1.2.4)$$

Carbon deposition will cause catalyst surface deactivation and shorten reformer tube life span by carbon blockage or hot spot at reformer tubes. Fortunately the overall carbon formation and carbon removal coexist in a dynamic equilibrium where the net effect depends on the following factors:

I. Gas Composition
II. Reforming pressure
III. Steam to carbon ratio
IV. Reformer temperature

Higher carbon number natural gas has higher carbon molar composition and therefore more prompt to carbon deposition on the catalyst surface especially at the top of the reformer tube where the methane concentration is the highest favoring methane cracking reaction (1.2.4). However since the gas composition varies from time to time, its contribution to carbon deposition are cancelled off by proper adjustment on the other three factors.

On the other hand, reforming pressure also play an important role in carbon deposition equilibrium since higher pressure suppress carbon deposition by favoring carbon removal rate. However higher pressure will shift the reforming equilibrium towards reactant side forming less hydrogen and carbon monoxide product due to the system equilibrium state reset to compromise the pressure increment by reducing its system pressure via reducing total number of gas molecule [8-10]. Operating the reformers at optimum pressure is thus needed to balance the tradeoff between carbon deposition control and syngas production. However since huge pressure altering is not practical for operating plant due to compressor capacity and plant pressure profile limitation. This research will only focus on studying the last two factors, which is the effect of S/C ratio and reformer temperature on synthesis gas production utilizing combined reforming of Steam-Methane Reforming (SMR) and Partial-Oxidation Reforming (POX).

Steam to carbon ratio (S/C ratio) is defined as the molar ratio of steam to carbon molar in the reformer feed. Excessive steam is feed to natural gas reformer to maintain a good steam to carbon ratio, (S/C) typically 3.5 to 5.0 to prevent carbon formation problem. In conjunction with operating pressure and temperature, S/C ratio also determine the hydrogen yield, $H_2/C0$ ratio of synthesis gas product and methane conversion, thus finding an optimum S/C ratio on natural gas reforming is also part of this research scope. Beside S/C ratio, reforming temperature also affects the syngas composition since methane reforming is a highly endothermic process (1.1.1). Higher temperature means more heat is available for the endothermic process and system equilibrium will shift towards product side [10].

The model of this research is based on the front-end operation of a methanol production plant. Using a similar reactor configuration at reforming unit, the daily operation gas data will be analyzed for operation optimization purposes. Current operation is to maintain a S/C ratio of 3:1 to avoid carbon deposition and safeguard the reformer, so this research is aiming to provide a feasibility study to operate with a lower S/C ratio that safe enough to prevent carbon formation while maintaining a good syngas ratio for methanol synthesis process.

In addition, a lower S/C ratio also allows plant operation to safe cost on raw water consumption and subsequently water demineralization plant chemical consumption cost. Currently the total raw water consumption rate of this methanol plant is about 160 Tons per hour (SMR alone consumed 80 Ton per hour), couple with frequent local water supply problem, this improvement could help leverage the raw water supply problem in the district.

1.3 Objectives and scope of study

1.3.1 Objectives

- Enhance understanding on natural gas reforming technology
- To develop a model of natural gas combined reforming using Hysis Simulation Software
- To study the effect of lowering S/C ratio on combine reforming to the syngas production
- To study the effect of reformer temperature on combine reforming to the syngas production
- To determine optimum S/C ratio and viz optimize operation of combine reforming

1.3.2 Scope of study

This research will focus mainly on setting up a model covering syngas production via combination of steam reformer and autothermal reformer using Hysis Simulation software. However, before the model can be set up, a thorough study and understanding of natural gas combined reforming from reaction chemistry and reaction kinetic is required. Thus the early stages will be concentrated on thereotical study of reforming reaction. Once sufficient knowledge is gathered on combined reforming, developing of the Hysis model will be the second stage. Then the last stage will require manipulation of operating parameter and steam to carbon ratio for process optimization.

CHAPTER 2

LITERATURE REVIEW AND THEORY

2.1 Steam Methane Reforming (SMR)

Pioneered by BASF in the first quarter of this century, Steam-Methane Reforming technology was introduced to replace coal gasification as the main hydrogen production source for ammonia and methanol synthesis. Reasons being for the replacement are abundant of natural gas supply available, cheaper process cost and hydrogen content of natural gas improved the yield of hydrogen per unit of carbon in the feedstock compared to coal. This technology was first used in 1931 by Standard Oil of New Jersey to produce hydrogen from off-gases at its Baton Rouge and Bayway refineries. The steam reforming reaction took place over catalyst in vertical tubes, which were supported, in parallel rows in a radiant furnace. The endothermic heat of reaction was supplied by burning fuel in the furnace.

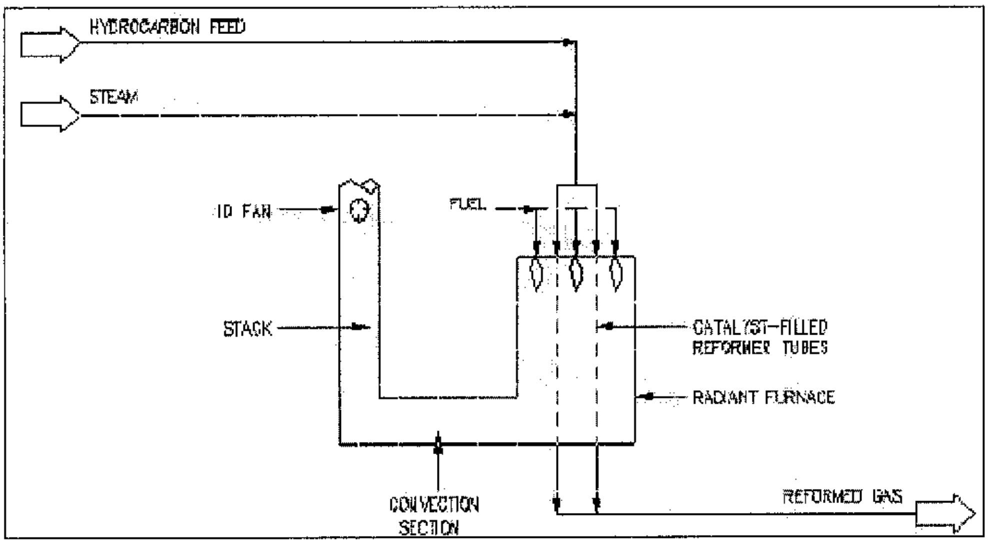


Figure 2.1: Steam-Methane Reformer configuration

The process was considerably improved by ICI, who developed the fundamental engineering data for the design of the furnace, improved the catalyst formulation and introduced the desulphurization step using zinc oxide. The process was used to produce hydrogen from off gases for coal hydrogenation plants, which ICI built in 1936 and 1940. The ICI technology was subsequently used in the development of the North American ammonia industry when plants were constructed at El Dorado, Baxter Springs, Etters, Sterlington and Calgary. All used natural gas, which contained mainly methane (80-90%) with low concentration of higher hydrocarbons.

Initially natural gas was not a readily available feedstock in UK before the discoveries in the North Sea, but as more refineries were built, other hydrocarbons such as naphtha, became increasingly available. It was apparent in the 1950s that if naphtha could be steam reformed economically; they would provide a cheap source of hydrogen for the manufacturing of ammonia.

In 1959 ICI started up the first large-scale pressure steam reformer using naphtha as feedstock, and this became the forerunner of over 400 plants subsequently licensed around the world in areas where natural gas was not available. From 1959 to date, development of the catalyst continued in order to allow plants to run at higher pressure and temperature, and with feedstock containing different hydrogen/carbon ratios. It also allowed feedstock with quantities of unsaturated and aromatic compounds to be reformed. It is until more recent year that the increasing of natural gas availability resulted in its use as a major source of reformer feedstock, and this trend is likely to remain so for a long time [1-2, 7].

The process chemistry of steam methane reforming is:

Endothermic Steam Reforming

$CH_4 + H_2O \Leftrightarrow CO + 3H_2$; ΔH^o_{298}= 206 KJ/mol (2.1.1)

$CH_4 + 2H_2O \Leftrightarrow CO_2 + 4H_2$; ΔH^o_{298}= 165 KJ/mol (2.1.2)

Exothermic Water-Gas shift reaction

$CO + H_2O \Leftrightarrow CO_2 + H_2$; ΔH^o_{298}= - 41KJ/mol (2.1.3)

The reforming reaction is strongly endothermic, so the forward reaction is favored by high temperature and low pressure. On the other hand, the shift reaction is exothermic and is favored by low temperature and largely unaffected by changes in pressure. To maximize the overall efficiency (and hence economics) of the conversion of carbon to carbon dioxide and the production of hydrogen, reformers are operated at high temperature typically 600-800°C and high pressure typically 30-40 Bar [6-7].

It can be seen that with methane, the stoichiometry requirement for steam per carbon is 1:1. However, it has been demonstrated that methane reforming at S/C ratio equal to 1:1 is not practical because all catalyst so far developed tend to promote carbon forming reactions under steam reforming conditions. These reactions can only be suppressed by using an excess of steam, with the result that the minimum S/C ratio is in the region of 1.7 [7], However, an excess of steam also promotes the reforming process itself and hence some advantage is derived from this necessity. In practice ratio of 3.0-3.5 are commonly used, but there can be economic attraction of using lower S/C ratios and now there is a trend in this direction.

2.2 Carbon formation

Carbon formation can occur from Bouduard reaction, carbon monoxide reduction and methane cracking processes as listed below:

Bouduard Reaction

$2CO \Leftrightarrow C + CO_2$ (2.2.1)

Carbon monoxide reduction

$CO + H_2 \Leftrightarrow C + H_2O$ (2.2.2)

Methane Cracking

$CH_4 \Leftrightarrow C + 2H_2$ (2.2.3)

The methane cracking reaction is endothermic and experiences increase in number of moles, hence it is favored by high temperature and low pressure. Because methane is consumed and hydrogen is produced in the reformer, the methane cracking is most likely to take place near reformer tube inlet. Temperature at the reformer tube outlet thermodynamically favor methane cracking but by then there is not so much of hydrogen and so little methane that there is no affinity for the coking reaction. This mean the composition is such that the reaction will proceed to the left (gasification by the hydrogen) rather than to the right (methane cracking) at the reformer outlet.

Both the Boudouard and CO reduction are exothermic and result in a decrease in moles, hence these reaction are favored by low temperature and high pressure. Since there is little or no CO at the inlet of the reformer, neither Bouduard and CO reduction reactions can take place where they are thermodynamically favored.

However, there can exist a region near the reformer inlet, where the temperature are low enough and concentration of CO and H_2 are high enough to favor Bouduard and CO reduction.

Rostrup and Nielsen [6,7] categorized three different types of carbon that is commonly detected in steam reformer. The three types of carbon are Pyrolitic carbon rock-like deposit, encapsulating carbon and whiskerlike filamentous carbon.

Pyrolitic carbon is formed via hydrocarbon feedstock thermal cracking, normally above 920K. In normal operating practice with active catalyst, the higher hydrocarbon will be converted in CO, CO_2 and H_2 by the time the process reaches 920K to form this type of carbon. Pyrolitic carbon is thus not a problem for steam reformer with active catalyst.

Furthermore, under typical reforming condition, there is no buildup of adsorbed hydrocarbon that can form at film that encapsulates and deactivates the catalyst. From this it can be concluded that the most effective carbon formation to steam reformer is the whisker type filament carbon.

Filamentous carbon cause no harm to the catalyst bed, however, it does causes activity loss by plugging catalyst pores and causing pressure drop over the reformer tubes. And since the plugged reformer tube is no longer cool by the endothermic reforming process, successive carbon built up might eventually cause tube metallurgical failure or ruptured.

Carbon formation is also favored by low reformer tube temperature. A study by ICI-KATALCO catalyst [11] shows that a 600°C, low-density carbon filament will form in large number. It can generate sufficient force inside pores of catalyst support to shatter catalyst pellet. At higher temperature between 650-700°C, a high-density platelet form of carbon will form at a prodigious rate, which will greatly adverse the reforming process by encapsulating most catalyst active surface. Fortunately any further increase in tube temperature >700°C will dramatically decrease the rate and quantity of carbon formation. Therefore it is critical to maintain operating condition at relatively high temperature between 700-800°C and with good S/C ratio to prevent this problem.

To determine the optimum S/C ratio to prevent Carbon formation, conventional approach is to experimentally measure the carbon formation boundary and operate the reactor under condition that prevents detection of carbon. According to Y.S, Seo, A Shirley, S.T Kolaczkowski [8].

> *The reactor temperature significantly affects the formation of solid carbon, C(s). It is generated at temperature of less than 850°C with S/C of 1.0 and at 1.0 bar reactor pressure. This implies that in order to avoid coke formation, the reactor temperature should be maintained at temperatures greater than 850°C. On the other hand, keeping the reactor temperature above 850°C is likely to damage the catalyst thermal durability. Therefore, it is necessary to change other operating parameters in order to suppress the coke formation in the temperature region below 850°C. The formation of solid carbon might cause by the following Boudouard reaction.*
>
> $$2CO \rightarrow C + CO_2$$
>
> *This is supported by the fact that CO_2 is generated only in the region in which C(s) exists (see Fig 2.2).*

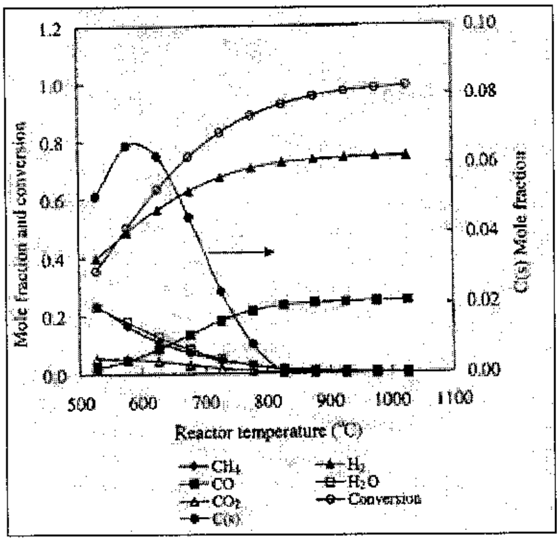
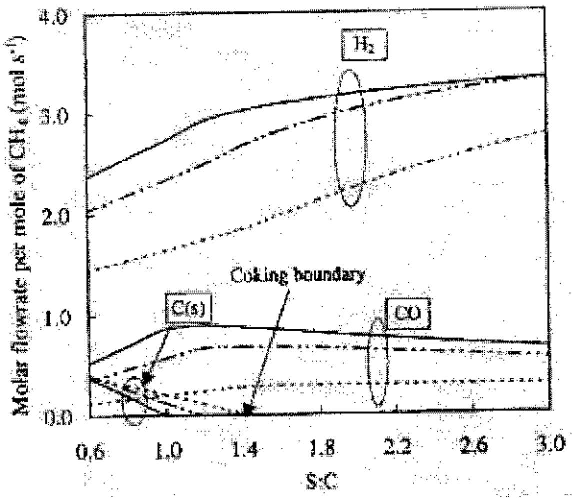


Figure 2.2: Effect of Reactor temperature on equilibrium composition and conversion is SMR reactor. Reactor Pressure 1Bar; S/C ratio: 1.0.

Their simulation work found that formation of C(s) is strongly affected by the value of S/C (see fig 2.3). The coking boundary is defined as the limit condition within which the coke is generated. The coking boundary in the SMR reactor moves towards lower S/C values as the reactor temperature is raised.

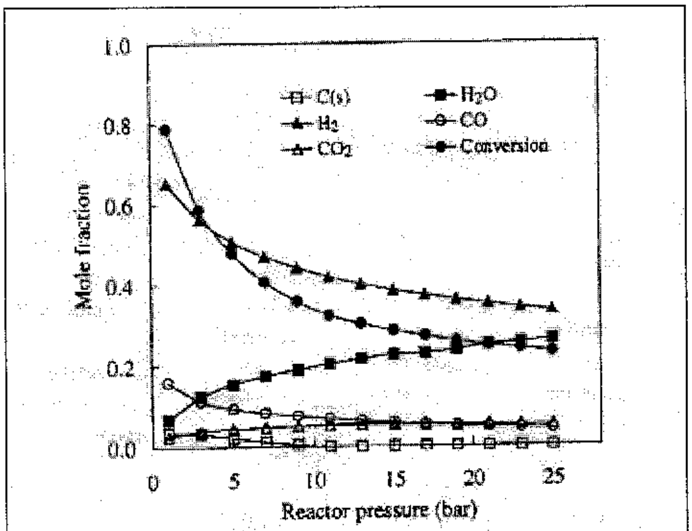


Effect of S:C on equilibrium compositions in SMR reactor. Reactor pressure: 1.0 bar, Reactor temperature: (- - -) 600 °C; (– · · –) 700 °C ; (—) 800 °C.

Figure 2.3: Effect of S/C on equilibrium composition in SMR reactor.

For example, if the temperature is increased from 600 to 800°C, the coking boundary moves from S/C of 1.4 to 1.0. These results demonstrate that formation of solid carbon can be avoided by increasing the reactor temperature and/or the S/C ratio. The maximum reactor temperature is restricted, however, by the thermal durability of the catalyst and the maximum S/C is limited according to the energy cost of the reactor system. A higher S/C ratio incurs a higher energy cost because of the extra steam generation required. The molar flow rate of H_2 is increased and increasing the S/C ratio decreases the molar flow rate of CO. This is an advantage with using a higher S/C ratio. The optimum S/C ratio of the SMR is found to be 1.9 or more, under operating condition of reactor pressure: 1 Bar, reactor temperature: 800°C.

Their research also further reveals that varying the operating pressure also effect the syngas composition (see figure 2.4). As the pressure is increased, the conversion and the mole fraction of H_2 and CO are rapidly reduced. However, carbon formation is drastically suppressed under high-pressure condition. Henceforth, carbon formation is estimated will unlikely to occur under S/C ratio 1.9 or more, reactor temperature at 800°C, reactor pressure of 40 Bar.



Effects of the pressure on the equilibrium compositions and conversion in SMR reactor. Reactor temperature, 700 °C; S:C ratio, 1.0.

Figure 2.4: Effect of Pressure on the equilibrium composition in SMR reactor.

2.3 Autothermal reforming

Autothermal reforming is a combination of partial oxidation and steam reforming process. Preheated pure oxygen will mix with steam and natural gas at the top of the reactor and partial oxidation of natural gas occurs. The chemistry involve are:

$CH_4 + ½O_2 \Rightarrow CO + 2H_2$; ΔH^o_{298}= -36 KJ/mol (2.3.1)

$CH_4 + 2O_2 \Rightarrow CO_2 + 2H_2O$; ΔH^o_{298}= -803 KJ/mol (2.3.2)

$CO + ½O_2 \Rightarrow CO_2$; ΔH^o_{298}= -284 KJ/mol (2.3.3)

$H_2 + ½O_2 \Rightarrow H_2O$; ΔH^o_{298}= -242 KJ/mol (2.3.4)

Notice that all reactions are exothermic, which means that heat is generated along the reaction. The term autothermal comes in when the exothermic heat of partial oxidation is used as the reaction heat for the endothermic steam reforming process at the bottom nickel catalyst bed. Hence, the reaction in the bottom nickel catalyst is same as the primary steam methane reforming.

The reactor is a refractory lined vessel. Therefore, higher pressure and temperatures can be applied than in steam reforming. Autothermal reactor is usually not applied on its own due to the high investment and operating cost (oxygen). Therefore it is frequently pair up with Steam reformer to produce syngas for ammonia or methanol synthesis. To produce syngas for ammonia synthesis, air is used in autothermal reformer to utilize the readily available nitrogen component in air. For methanol synthesis, pure oxygen is used to produce syngas with good proportion of hydrogen, carbon monoxide and carbon dioxide gas.

Autothermal reformer brings advantage of producing a lower H_2/CO ratio syngas, which favor downstream methanol synthesis process. Careful selection of operating conditions and proper mixing of the process inlet stream prevent carbon formation reactions from occurring in the combustion zone.

CHAPTER 3

METHODOLOGY

This study was done based on front-end combine reforming unit of a methanol production plant. The reforming process start from feeding about 43200 to 57600 Nm^3/hr of natural gas to desulphurization process at sulphur catch-pot D-101. The temperature and pressure for this desulphurization is at 387°C and 40 Bar. Sulphur removal process is crucial since it will poison the reformer nickel catalyst. The sulphur free natural gas is then divided into 2 streams based on system design ratio of 52:48 split, the larger portion is routed to a pre-reformer D-103 to steam reform most higher hydrocarbon: ethane, propane, butane and pentane. Methane slippage at this stream is reducing from 90% to about 75%. Gases at pre-reformer outlet undergo further reforming with at primary steam reformer B101. Steam and gases from pre-reformer is mixed typically at S/C ratio of 3:1 and undergo further reforming under the present of nickel catalyst. The typical methane slippage at steam reformer outlet is reduced from 75% to about 12 to 15%.

B101 outlet stream is combine with the earlier 42% portion fresh gas and mixed with pure oxygen gas from air separation unit (ASU), and undergo partial oxidation reforming in secondary autothermal reactor R101. Exothermic partial oxidation reactions upgrade the reaction heat to about 1200°C to 1300°C at the combustion zone of the reactor. The steam reforming further takes place in the R101 catalyst bed and causing the overall reaction to be endothermic. As the result of this phenomenon, R101 outlet temperature is dropped from 1200°C at top of reformer to 920°C to 945°C at the reformer outlet. The final methane slippage at R101 outlet is usually observed between 1.5 to 3.5%. Indicating high efficiency of overall methane conversion.

A HYSYS simulation model based on the pre-reformer D-103, primary steam reformer B101 and secondary autothermal reactor R101 were developed to allow further study on the gas-reforming unit. Analysis has commenced using the developed model to study the effects of varying S/C ratio and the reactor temperature on primary steam reformer B101 towards the steam reformer B101 and R101 overall syngas composition. Simulation data were tabulated and analyze in Microsoft Excel.

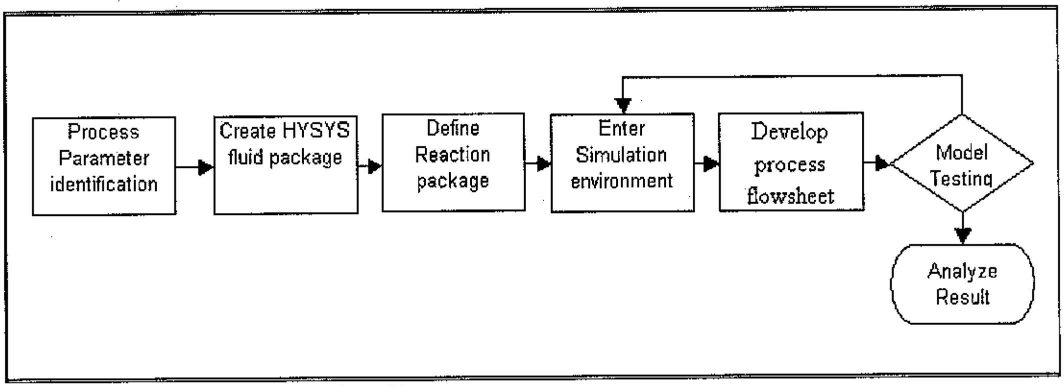


Figure 3.1: Simulation Process Flow Chart

Before developing the simulation model, the initial work was done to identify all process parameter and unit-operating condition such as feed temperature, pressure and composition. Upon developing the HYSYS model, since all reactant are in gas phase, the fluid package selected for the simulation is the Soave-Redlich-Kwong Equation of state since it is better in predicting vapor pressure in pure component or mixture compare to other available equation of states.

The chemical component of the reforming processes were inserted to the fluid package and all involved chemical reaction of the reforming processes is defined according to the chemical reaction stoichiometry at the simulation basis manager page under the reaction tab. The simulation model is then developed within the simulation environment of HYSYS. The thermodynamic equilibrium in a reformer reactor is calculated making use of HYSYS Gibbs reactor. Gibbs reactor calculates the equilibrium composition of the outlet stream by minimizing the total Gibbs free energy of the reaction system. Therefore, giving a reasonable estimation of equilibrium composition at constant temperature and pressure because minimum Gibbs free energy correspond to equilibrium state at constant temperature and pressure for any real, spontaneous process [12]. Finally, all operation stream and unit operation such as mixer is attached to the reactor based on plant configuration. The simulation model is attached in the figure below and the workbook simulated at S/C ratio 3:1 is attached to the appendix.

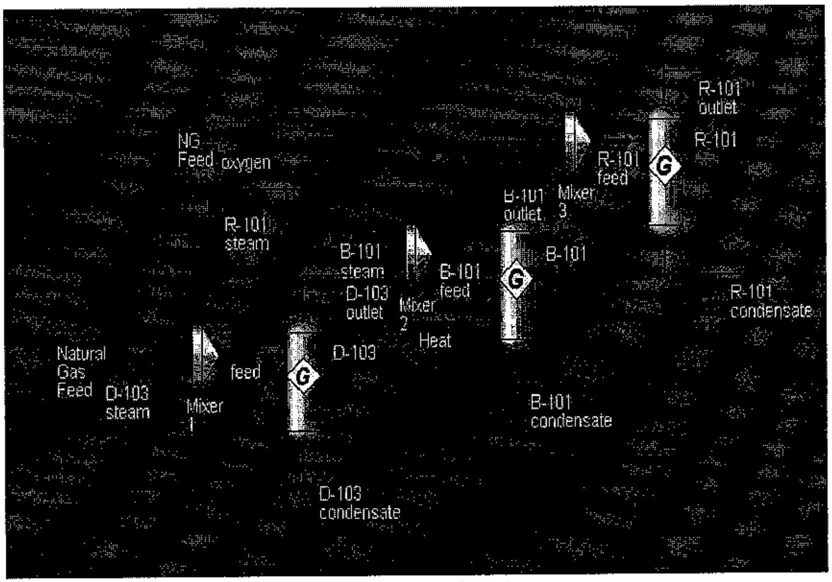


Figure 3:2: HYSYS Simulation model on reforming system

CHAPTER 4

RESULTS AND DISCUSSION

Upon the completion of the simulation model, two factors as listed below will be tested using HYSYS to study its effect to the syngas composition at steam reformer and autothermal reformer:

1. Varying S/C ratio from 1 to 10 at Primary steam reformer
2. Varying B101 reactor temperature at Primary steam reformer

One point worth to mention here is that S/C ratio and temperature factor were not tested on autothermal reactor. This is because these factors are not the dominant factor in partial oxidation reaction (2.3.1-4). A more proper factor that significantly affects the partial oxidation reforming in autothermal reactor will be oxygen to natural gas ratio, O_2/CH_4 but study on this factor is beyond the scope of this project.

However, since the combined reforming system studied in this project was designed to produce syngas for methanol synthesis process. The autothermal reformer was coupled with steam methane reformer to maximize production of carbon dioxide and carbon monoxide from partial oxidation reaction (2.3.1-4). Since 52% of R101 feed is from SMR outlet, thus changes in primary steam reformer performance interactively affect the performance of autothermal reformer.

In another words, varying the mentioned factors to syngas production at primary steam reformer will affect the syngas composition at both primary and secondary reformer. The effect of these factors are analyzed and elucidated at following discussion.

4.1 Steam Carbon Ratio Analysis

For the S/C ratio analysis, natural gas carbon number was calculated to be 1.1593. The operating condition of the reforming system is given below:

I. Natural gas temperature: 400°C
II. Natural gas pressure: 40 Bar
III. Steam temperature: 550°C
IV. Steam pressure: 40 Bar

The S/C ratio of B101 furnace was varied from 1 to 10. No adjustment has been made to R101 operating parameter but since R101 gas feed is partially from B101 reactor, any adjustment on B101 reactor will also affect R101 reactor performance. Below are the data of component molar flowrate at the outlet of primary steam reformer B101 and secondary reformer R101.

Table 4.1: Molar composition of B101 reactor at various S/C ratio.

S/C	Molar flow	Methane	CO	CO2	Hydrogen	Steam
1	7680.0	386.3	920.6	302.6	5327.1	743.4
2	9186.0	444.6	902.1	262.7	6734.8	842.4
3	10700.0	500.8	877.4	232.2	8161.0	929.8
4	12210.0	554.3	847.4	206.3	9592.8	1008.5
5	13730.0	606.9	815.6	185.4	11039.1	1081.9
6	15250.0	658.8	782.3	167.8	12490.6	1149.9
7	16710.0	705.2	745.3	152.4	13896.3	1209.8
8	18300.0	755.8	713.7	139.6	15413.7	1277.3
9	19800.0	801.9	677.2	127.5	16858.9	1334.5
10	21400.0	851.7	644.1	117.3	18392.3	1395.3

Table 4.2: Molar composition of R101 when B101 Subjected to S/C adjustment.

S/C	Molar flow	Methane	CO	CO2	Hydrogen	Steam
1	13180.0	0.5	2672.7	355.9	8469.6	1542.6
2	14560.0	1.8	2629.0	342.2	9927.9	1522.2
3	16170.0	5.5	2628.3	338.0	11532.0	1529.7
4	17780.0	13.8	2623.7	336.0	13129.6	1541.5
5	19370.0	29.1	2611.8	331.2	14701.4	1559.3
6	20950.0	52.2	2593.8	326.8	16252.8	1588.0
7	22510.0	82.4	2568.9	321.9	17777.3	1623.0
8	24060.0	118.4	2539.3	315.2	19285.2	1665.0
9	25610.0	158.3	2507.2	307.3	20787.1	1713.3
10	27140.0	200.8	2469.7	301.3	22268.8	1761.4

From the simulated result of combined reforming, graph of major component molar flowrate at reactor outlet versus S/C ratio were plotted in order to analyze the trending curve for each major component when B101 subjected to S/C adjustment.

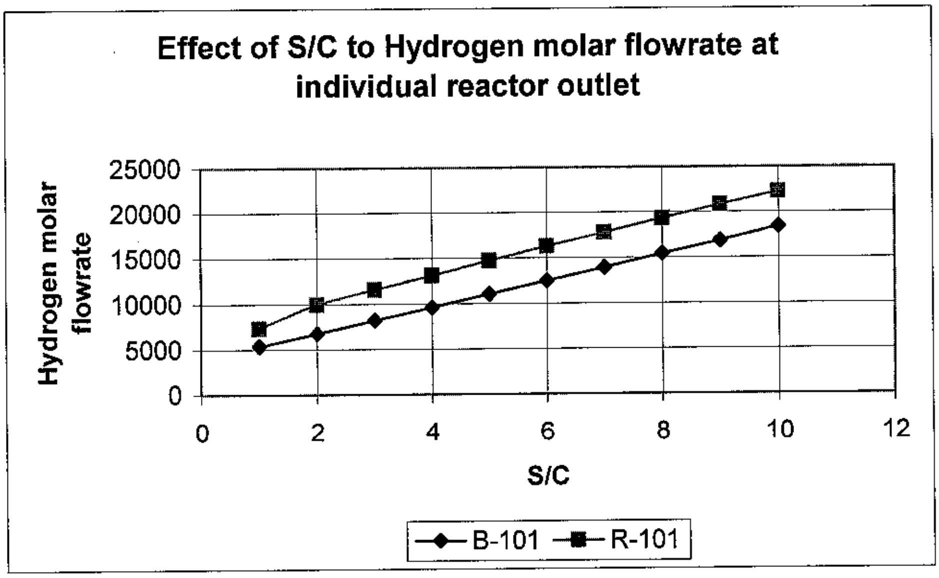


Figure 4.1: Effect of S/C ratio to Hydrogen composition

As shown in figure 4.1, the amount of hydrogen mole increase with higher S/C ratio subjected to B101. This is expected since excessive of steam will push the reaction towards the hydrogen and carbon monoxide product side by equation (2.1.1) and

(2.1.2). This is in agreement with the reaction kinetic mechanism (1.2.1 a-e) suggested by Rostrup-Nielsen [6,7] whereby steam molecule will dissociate to form hydrogen and oxygen atom to react with hydrocarbon in steam reforming process. Thus, incremental of S/C ratio actually causing more steam molecule to dissociate and forming more hydrogen gas molecules. Typical operation of steam reformer often yields a 60-70% of hydrogen gas.

Large amount of hydrogen gas generated from primary steam reformer B101 will reinforce hydrogen gas yield in secondary partial oxidation reformer R101 and eventually forming a large total amount of hydrogen gas product at R101 outlet. The amount of hydrogen gas production is about 8161.0 kmol/hr when B101 operates at S/C ratio of 3:1 but decrease to 6734.8 kmol/hr when B101 operates at S/C ratio of 2:1 as depicted in Table 4.1. A total of 11532.0 kmol/hr of hydrogen gas is produce at R101 outlet when B101 operates at S/C ratio of 3:1 but the production decrease to 9927.9 kmol/hr when B101 operates at S/C ratio of 2:1 as depicted in Table 4.2. This gives at percent reduction of 17% at B101 and 14% at R101, which mean hydrogen yield are 17% less at B101 outlet and 14% less at total hydrogen gas yield when B101 operates at S/C of 2:1 compare to operation of B101 at S/C of 3:1.

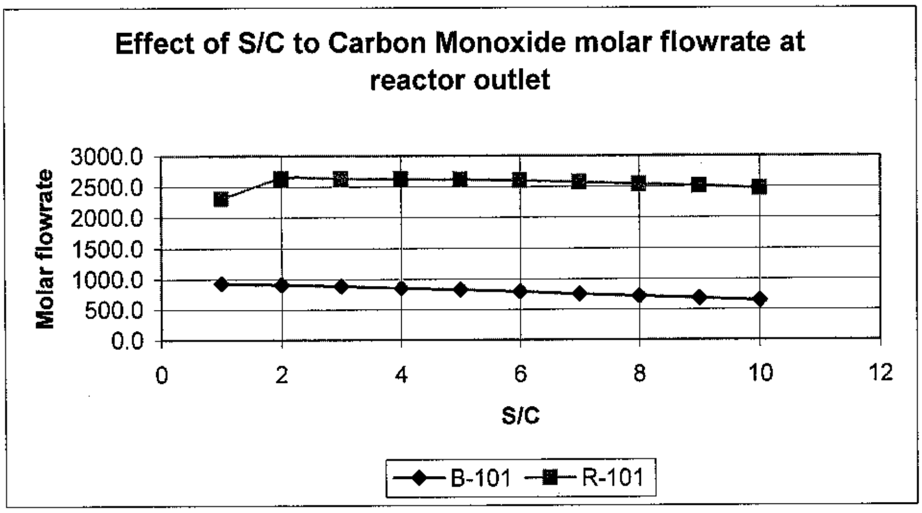
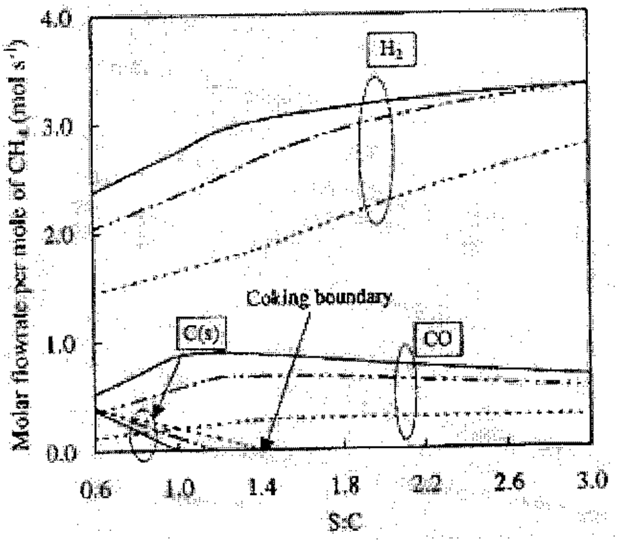


Figure 4.2: Effect of S/C to Carbon Monoxide composition.

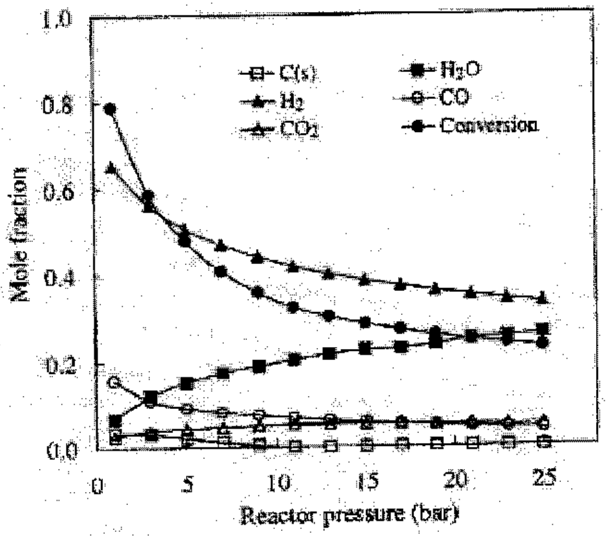
The amount of carbon monoxide produced from B101 decreases with increasing S/C ratio as shown in Figure 4.2. However, this result does not agree with Le Châtelier's equilibrium principal in the sense that more carbon monoxide should be formed when S/C ratio is raised. This is because as more steam reactant is feed into the reforming process, it will consume more methane reactant to produce more hydrogen and carbon monoxide product. Moreover, exothermic water gas-shift reaction also shifts equilibrium toward formation of more carbon monoxide gas.

According to Y.S.Seo, A Shirley, S.T.Kolaczkowski [8], when the S/C ratio is raised, the molar flow rate of H_2 is increased but the molar flow rate of carbon monoxide is decreased. This finding was experiment determined under the condition of 1.0 bar reactor pressure (Figure 4.3). According to Le Châtelier's equilibrium principal, when the pressure is increase, carbon monoxide molar content will reduce (Figure 4.4). Reduction of carbon monoxide molar will cause lower yield on methanol synthesis, thus higher S/C ratio and pressure should be avoided in order to produce sound amount of methanol product.



Effect of S:C on equilibrium compositions in SMR reactor. Reactor pressure: 1.0 bar. Reactor temperature: (- - -) 600 °C; (- · · -) 700 °C ; (—) 800 °C.

Figure 4.3: Effect if S/C on equilibrium in SMR reactor.

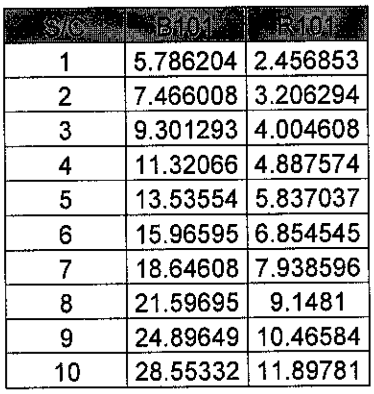


Effects of the pressure on the equilibrium compositions and conversion in SMR reactor. Reactor temperature, 700 °C; S:C ratio, 1.0.

Figure 4.4: Effect of pressure on equilibrium in SMR reactor

The amount of carbon monoxide gas in R101 reactor is higher than B101 because extra carbon monoxide is being produce by partial oxidation reforming in R101. Operating at S/C ratio of 2:1 instead of 3:1 gives increment of about 3% of CO formation at B101. This coupling effect of hydrogen reduction and increase of carbon monoxide in overall will reduce hydrogen to carbon monoxide ratio in the syngas product when lowering the S/C ratio at B101. However, molar ratio H_2/CO of 3.2 still fulfills the requirement of methanol synthesis (molar ratio H_2/CO of 2:1) as depicted in Table 4.3.

Table 4.3: Stoichiometry H_2/CO ratio at various S/C



S/C	B101	R101
1	5.786204	2.456853
2	7.466008	3.206294
3	9.301293	4.004608
4	11.32066	4.887574
5	13.53554	5.837037
6	15.96595	6.854545
7	18.64608	7.938596
8	21.59695	9.1481
9	24.89649	10.46584
10	28.55332	11.89781

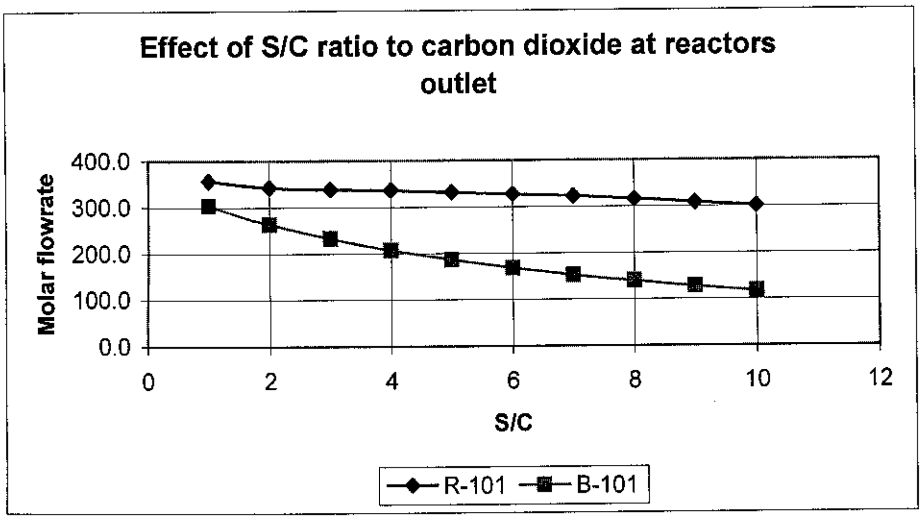


Figure 4.5: Effect of S/C to carbon dioxide composition

In terms of carbon dioxide formation, increasing S/C ratio reduces the formation of carbon dioxide at B101 outlet. The same trend was observed occurs to R101 except at slower rate. This is due to the oxidation of natural gas that take place in R101 producing carbon dioxide.

Reduction of carbon dioxide in the primary steam reformer is expected since the water-gas shift reaction (reaction 1.1.2), is a slight exothermic reaction. Thus incremental of S/C ratio will then increase the reformer temperature and causing the equilibrium to shift towards the reactant side. Thus more carbon dioxide gas will react with hydrogen gas to form carbon monoxide and steam. Concerning carbon dioxide reduction when S/C ratio increases, this phenomenon actually favors methanol synthesis process. This is due to less water byproduct formed when carbon dioxide concentration is small, therefore reducing the load for separation utilities. This argument is illustrated in equation (4.1) and (4.2) below.

$$CO + 2H_2 \Leftrightarrow CH_3OH \qquad (4.1)$$

$$CO_2 + 3H_2 \Leftrightarrow CH_3OH + H_2O \qquad (4.2)$$

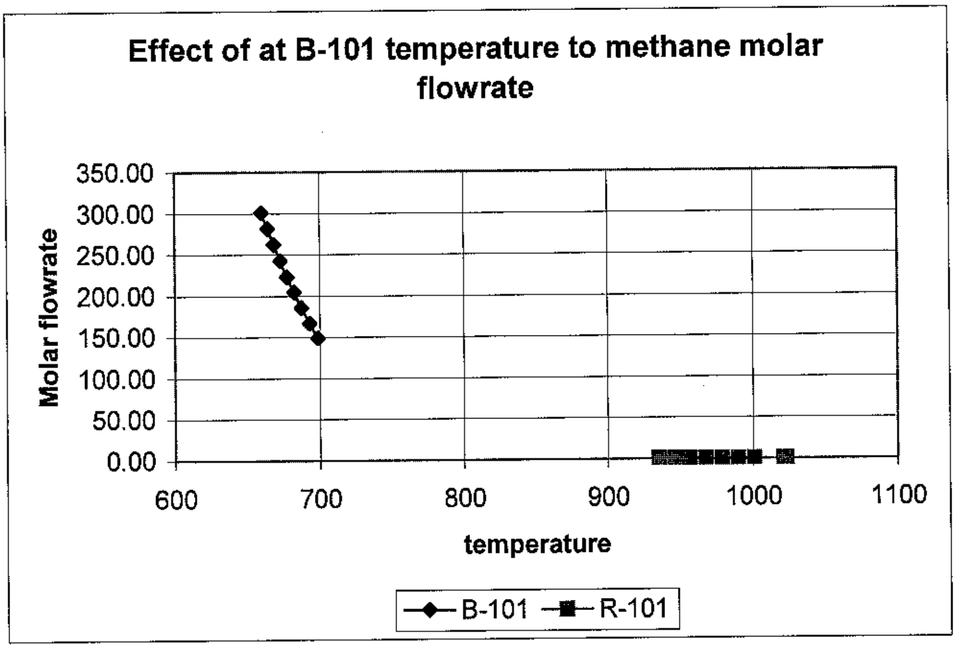


Figure 4.6: Effect of steam temperature at B101 to methane composition at both reformer outlets.

The steam inlet temperature was varied to give a corresponding B101 outlet temperature range between 650 to 700°C. As the reaction temperature at B101 increases, the amount of methane at both reformers outlet decreases as shown in Figure 4.6. Steam methane reforming is an endothermic process and thus favors by high temperature as stated in Le Châtelier's equilibrium principal. This is because higher temperature introduces more heat into the equilibrium system, this heat sources can be treated as if it were the reaction's reactant in endothermic reaction. Hence, the system will shift its equilibrium producing more product by consuming the extraneous heat source to re-establish system equilibrium. Equation (4.3) below explains this process.

Endothermic reaction: Reactants + Heat ⇔ Products (4.3)

In real operation, routine B101 operation is maintained at temperature of 800 to 850°C. Despite the error of HYSYS estimation on B101 temperature, nevertheless it does show higher temperature favors conversion of methane in the reforming processes.

Figure 4.6 also shown that partial oxidation plus steam reforming reaction in R101 completely reform the methane component in R101 natural gas feed stream. R101 natural gas feed stream here refers to the 52% reformed gas from steam reformer B101 outlet plus 42% of fresh feed natural gas from front end. The complete reforming is due to the highly exothermic reaction heat from partial oxidation process in R101 has the capability to supply larger amount of heat to the second level steam reforming at R101 catalyst bed. In real operation, typical methane slippage at R101 outlet is about 1.5 to 3%.

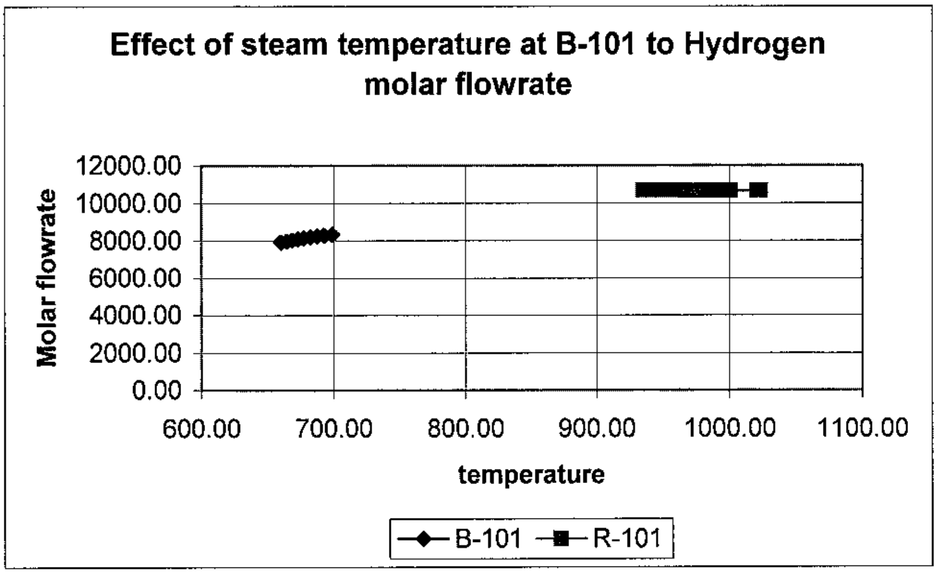


Figure 4.7: Effect of B101 temperature to hydrogen composition at both reformers outlet.

Refer to Figure 4.7, higher temperature favors steam reforming conversion and producing more hydrogen at B101. This is again is due to higher temperature supplies more reaction heat to the endothermic steam reforming process. The net effect of heat addition causes the system to re-establish equilibrium by shifting equilibrium towards product side via producing more hydrogen gas product.

The total hydrogen gas product is slightly reduces at R101 outlet as shown in Figure 4.7, due to slight exothermic water-gas shift reaction as stated in equation (2.1.3). Highly exothermic partial oxidation reaction at autothermal reformer causing some hydrogen and carbon dioxide being consume to produce more carbon monoxide and steam. This is in line with Le Châtelier's equilibrium principal, because for exothermic process, the heat source can be treated as if it were the product of the reaction.

$$\text{Exothermic: Reactants} \Leftrightarrow \text{Products} + \text{Heat} \qquad (4.4)$$

Thus high temperature of partial oxidation process at R101 inlet is supplying heat for the water-gas shift reaction and causing the system to shift equilibrium towards the reactant side. However the reduction rate is rather constant as shown in Figure 4.7.

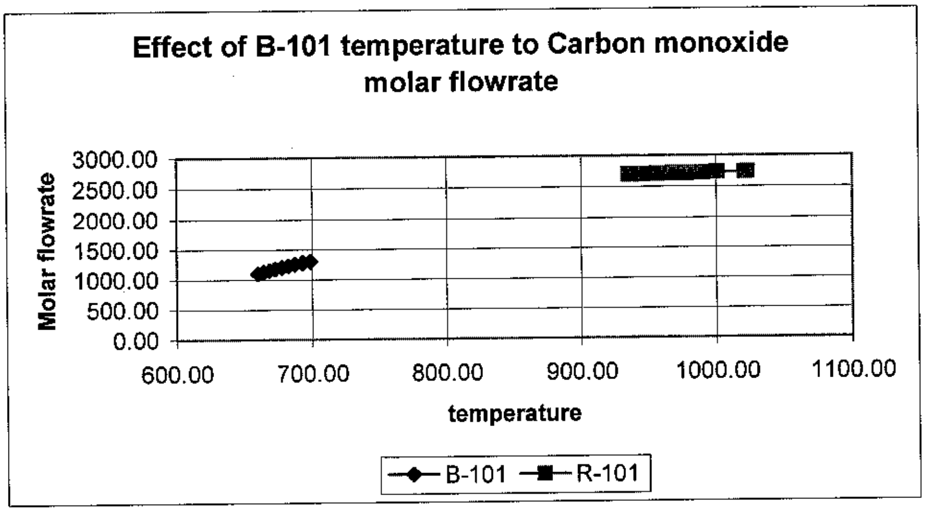


Figure 4.8: Effect of B101 temperature to carbon monoxide composition at both reformers outlet.

Figure 4.8 shows that as temperature increases, the carbon monoxide production will also increases. Consecutively, numbers of carbon monoxide in R101 also increase because partial oxidation process reinforces the production of carbon monoxide gas. Moreover, exothermic water gas shift process leads to an increase in the carbon monoxide component due to equilibrium shift favoring reactant side in R101 reactor.

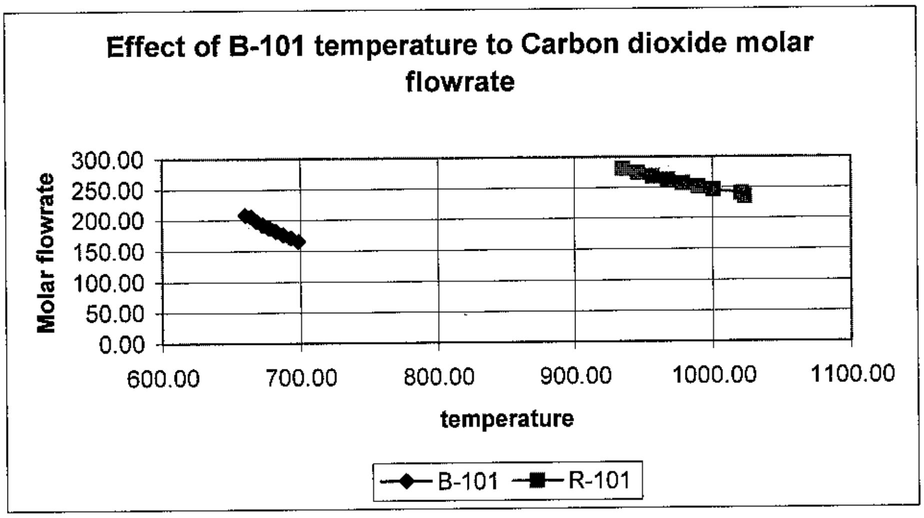


Figure 4.9: Effect of B101 temperature to carbon dioxide composition at both reformers outlet.

As the temperature of B101 increases, the amount of carbon dioxide production from both reformers decreases as represented by Figure 4.9. For B101 reformer, reduction of carbon dioxide component is due to the exothermic nature of water-gas shift reaction. Thus higher temperature means higher heat content and the water-gas shift will favors the reactant side. In R101 reformer, the same phenomenon occurs except complete oxidation of natural gas is actually producing carbon dioxide, thus the overall carbon dioxide production in R101 is higher than the amount produced in B101.

Thus overall, maintaining high reactor temperature at B101 steam reformer helps to improve methane conversion and as a result of this, methane slippage is reduce with more hydrogen and carbon monoxide gas produced. Carbon dioxide gas however, are produce less as B101 temperature increases. From table 4.4 and 4.5, the highest reactor outlet temperature for B101 and R101 are 698.52 and 1023.40°C respectively. In real operation, B101 outlet temperature is usually between 760 to 800°C and R101 outlet temperature prior waste heat boiler is between 920 to 960°C. Henceforth it can be estimated that even operated at S/C ratio of 2.5:1, if B101 reactor temperature is maintain at 800°C region, good methane conversion is maintained and producing the desired amount of hydrogen and carbon monoxide gas for direct methanol synthesis. With less carbon dioxide gas produce at higher B101 temperature, it can help to improve selectivity of CO rather than CO_2 methanol synthesis.

4.3 Pressure effect

Generally pressure effect also contributes largely to the equilibrium of the reforming process. Le Châtelier's principal stated: for any system at equilibrium, if a disturbance of change in temperature, pressure, or the concentration of one of the components, the system will shift its equilibrium position to a direction that minimizes or reduces the effect of disturbance. Therefore an increase in system pressure will disturb the equilibrium of the system and forcing gas molecule to occupy a smaller volume. A system can reduce its pressure by reducing the total number of gas molecules to occupy a smaller volume.

Therefore, since steam reforming and water-gas shift processes involve reaction that producing more total number of gas molecule, reducing the system pressure will cause the system to increase its total pressure to re-establish equilibrium. So, the system will shift reaction side that favors the formation of hydrogen gas, carbon monoxide and carbon dioxide. However, even thought lower pressure operation will give us more optimum condition in producing more synthesis gas, but major adjustment in reactor operating pressure will disturb the plant line pressure difference profile and disturb the backend methanol synthesis process perhaps incurring higher compression cost because the pressure in the methanol synthesis loop is optimize at

80 Bar for the reactor. Thus, to avoid incurring more capital cost and technical modification problem, the front end reforming process system pressure is maintain at constant 40 Bar in this study.

4.4 Economic analysis

Table 4.6: Steam consumption rate at various S/C ratios.

S/C ratio	Gas Molar (kgmole/hr)	Carbon Molar (kgmole/hr)	Steam Molar (kgmole/hr)	Steam Flow (Ton/hr)
1	1400	1623.02	1623.02	29214.36
2	1400	1623.02	3246.04	58428.72
3	1400	1623.02	4869.06	87643.08
4	1400	1623.02	6492.08	116857.44
5	1400	1623.02	8115.1	146071.8
6	1400	1623.02	9739.12	175304.16

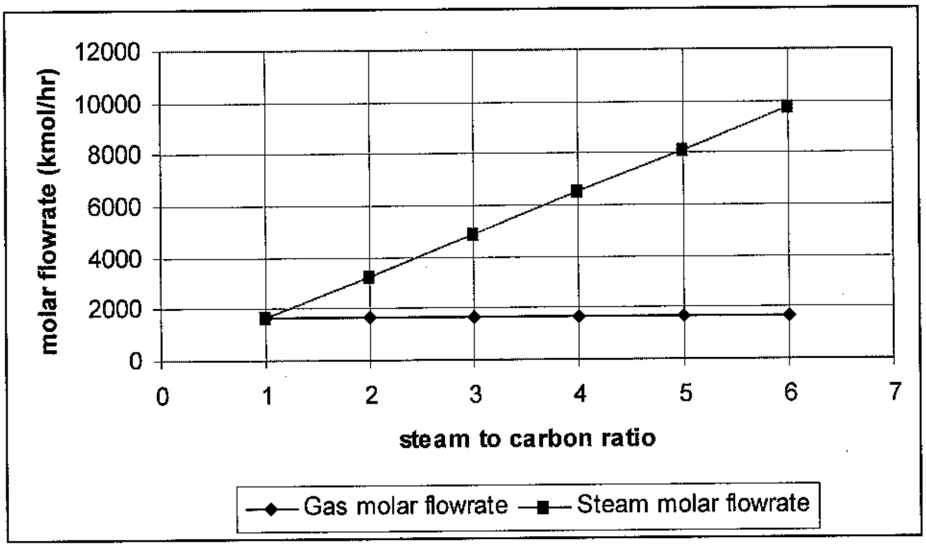


Figure 4.10: Relation between steam to gas molar flowrate as S/C ratio increases

In this project, natural gas carbon number is assumed as 1.1593. Based on the calculation in the table above. About 87 Ton/hr of steam is needed for primary steam reformer B101 feed to achieve S/C ratio of 3:1 to prevent carbon formation in steam reformer B101. The amount of steam increases proportionately relative to amount of gas as shown in Figure 4.10, thus our objective is to find the optimum S/C ratio and thus giving the optimum amount of steam to be used in order to achieve the S/C ratio. Based on most literature studies, under operating condition of 40 bar pressure and around 780°C, critical steam to carbon ratio to prevent carbon deposition is about 0.6-3.0 (Y.S, Seo, A Shirley, S.T Kolaczkowski). Other literature finding such as Twiggs [7] estimated the minimum S/C ratio is in the region of 1.7 and Jacod A Moulijn [1] estimates S/C between 2.5 to 4.5. Henceforth possibility of lowering down S/C ratio to 2:1 could save plant operation from consuming excessive raw water at about reduction of 33.4% from 87 Ton/hr to 58 Ton/hr, equivalent to saving 30 tons of raw water per hour or 720 Ton/day, provided the syngas process does not get affected. Such improvement could save the plant operation from reducing raw water consumption cost, Demin water chemical consumption cost and perhaps leverage the raw water supply problem in the district.

From the analysis, a rather conservative suggestion would be to study feasibility to operate B101 with S/C ratio of 2.5:1 instead of 3:1, then the potential cost saving from this improvement would be consuming about 73 TPH of steam instead of about 87 TPH. Saving about 14 TPH of steam and its associated BFW treatment cost.

4.5 Limitation of the simulation model

For the simulation model, all 3 reformers are model as Gibbs reactor since specific reaction kinetic of the reforming process was not known. Gibbs reactor works by finding the equilibrium state with the lowest Gibbs free energy. It appears to be akin to finding all the possible equilibrium reactions and allowing them all to equilibrate. However by not taking account of the catalyst activity, the accuracy of the result is severely affected. For instance, D-103 in the methanol plant operation is a simple tubular reactor utilizing highly active nickel catalyst to reform most of the higher hydrocarbon at low temperature of 400°C and 40 Bar Pressure. Such condition was not able to include in Gibbs reactor and thus causing reverse reaction of methane reforming into methane forming when subjected to low temperature and high pressure condition.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

As a conclusion to this final year research project, the objective of enhancing understanding on natural gas reforming technology, particularly on combined reforming of Steam Reforming plus autothermal partial oxidation reforming has been achieved and revised greatly by continuous literature and research findings.

Thanks to the information available from a local methanol plant on combined reforming of natural gas, a simulation model was developed to study the effect of lowering S/C ratio from 3:1 to a lower value on syngas production. Aiming to study the possibility to improve reforming operation by safe cost on steam consumption. However, the developed simulation model did not consider the effect of reaction kinetic rate and catalyst activity. Thus leaving ample space for further model improvement to enhance process estimation accuracy.

From the simulated result analysis, higher S/C ratio increases Hydrogen production, decrease CO and CO_2 production and incur higher steam cost. Reduction of CO and CO_2 is not favorable since the production of methanol is directly proportionate to the amount of these two important chemical components. From the result as well, it can be estimated that if the methanol plant were to operate Primary reformer with S/C of 2:1 instead of 3:1, it will lead to 17% reduction of hydrogen gas production, 3% increment of CO and about 1.2% increment of CO_2 production. The H_2/CO ratio will decrease to 3.02 rather than 4 at S/C ratio of 2:1. But nevertheless the ratio still meets the requirement of methanol synthesis (H_2/CO ratio= 2:1).

B101 Temperature analysis shows that at higher temperature, it can improve methane conversion, producing more hydrogen and carbon monoxide component and lesser carbon dioxide formation. This favors methanol synthesis since reaction between carbon dioxide with hydrogen will yield by product water but reaction between carbon monoxide and hydrogen will directly yield methanol product.

Lastly, since carbon boundary must be experimentally measure, thus estimation based on researcher's finding is used in this project to estimate the minimum S/C ratio that can safeguard carbon formation problem. According to Y.S.Seo [8], optimum S/C ratio estimated is 1.9 or more at reactor pressure of 1 bar, reactor temperature of 800°C. Twiggs [7] estimated minimum S/C ratio is in the region of 1.7. Jacod A Moulijn [1] estimates S/C between 2.5 to 4.5. A rather conservative suggestion would be to operates steam reformer with S/C ratio of 2.5:1 since it could save cost the operation about (87TPH-73TPH) 14 Tons per hour of steam and its associated boiler feed water (BFW) treatment cost.

Recommendation on future work would be to experimentally determine the reaction kinetic rate and take into consideration of catalyst activity and the effect of catalyst poisoning. This will enhance the estimation the reforming process and accurately determine the minimum S/C ratio for reforming process and provide a more solid basis to determine the optimum S/C ratio. Also, there is still more to study on natural gas combined reforming, for instance like the effect of oxygen to methane ratio.

REFERENCES

[1] Jacod A Moulijn, Michiel Makkee and Annelies van Diepen. 2001, *Chemical Process Technology*, New York, John Wiley & Sons.

[2] Harold Gunardson. 1998, *Industrial Gases in Petrochemical Processing*, New York, Marcel Dekker Inc.

[3] Sunggye Lee. 1997, *Methane And Its Derivatives*, University of Akron, Ohio.

[4] Alan G.Lucas. 2000, *Modern Petroleum Technology Vol 2 Downstream*, New York, John Wiley & Sons.

[5] Katalin Hangos and Ian Cameron. 2001, *Process Modelling and Model Analysis*, Academic Press, London.

[6] R.J.Farrauto and C.H.Bartholomew. 1997, *Fundamentals of Industrial Catalyst Processes,* Blackie Academic & Professional, London

[7] Martyn V.Twigg. 1996, *Catalyst Handbook 2nd Edition*, Manson Publishing, England

[8] Y.S.Seo, A. Shirley, S.T.Kolaczkowski, *J. power sources* 108 (2002) 213-225.

[9] A.L. Larentis, Neuman Solange de Resende, *Applied catalysis A*: General 215 (2001) 211-224.

[10] Brown, Lemay & Bursten, 1997 *Chemistry the Central Science 7th Edition*, Prentice Hall International Inc.

[11] ICI KATALCO SYMPOSIUM – Malaysia 1991 on reforming catalyst.

[12] Jack Winnick, 1997, *Chemical Engineering Thermodynamics*, John Willey & Sons, Inc.

Appendix

Extracted data for S/C ratio analysis from HYSYS

S/C	B-101	Inlet	Outlet
1	methane	0.396425	5.03E-02
	ethane	1.83E-05	3.07E-07
	propane	2.76E-09	5.12E-12
	I-butane	7.44E-16	1.36E-23
	n-butane	1.02E-15	2.77E-23
	I-pentane	1.10E-22	1.97E-32
	n-pentane	4.87E-23	1.28E-32
	CO	1.12E-04	0.119876
	CO2	2.59E-02	3.94E-02
	hydrogen	3.36E-02	0.693627
	h20	0.54387	9.68E-02
	n2	9.56E-49	7.07E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	5.06E-25

S/C	R-101	Inlet	Outlet
1	methane	0.163689	3.93E-05
	ethane	6.62E-03	5.42E-03
	propane	4.04E-03	3.30E-03
	I-butane	8.94E-04	7.32E-04
	n-butane	7.83E-04	6.41E-04
	I-pentane	3.13E-04	2.57E-04
	n-pentane	2.28E-04	1.87E-04
	CO	8.69E-02	0.202783
	CO2	3.01E-02	2.70E-02
	hydrogen	0.502922	0.642613
	h20	9.76E-02	0.11704
	n2	5.13E-49	8.19E-49
	Carbon	0	1.00E-45
	oxygen	0.105946	9.69E-18

S/C	B-101	Inlet	Outlet
2	methane	0.396425	4.84E-02
	ethane	1.83E-05	2.73E-07
	propane	2.76E-09	4.23E-12
	I-butane	7.44E-16	7.91E-24
	n-butane	1.02E-15	1.61E-23
	I-pentane	1.10E-22	9.81E-33
	n-pentane	4.87E-23	6.37E-33
	CO	1.12E-04	9.82E-02
	CO2	2.59E-02	2.86E-02
	hydrogen	3.36E-02	0.733162
	h20	0.54387	9.17E-02
	n2	9.56E-49	7.68E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	4.64E-25

S/C	R-101	Inlet	Outlet
2	methane	0.148143	1.27E-04
	ethane	5.80E-03	4.82E-03
	propane	3.53E-03	2.94E-03
	I-butane	7.82E-04	6.50E-04
	n-butane	6.86E-04	5.70E-04
	I-pentane	2.74E-04	2.28E-04
	n-pentane	1.99E-04	1.66E-04
	CO	7.46E-02	0.180563
	CO2	2.30E-02	2.35E-02
	hydrogen	0.556682	0.681859
	h20	9.36E-02	0.104548
	n2	5.83E-49	8.31E-49
	Carbon	0	1.00E-45
	oxygen	9.28E-02	7.59E-19

S/C	B-101	Inlet	Outlet
3	methane	0.396425	4.68E-02
	ethane	1.83E-05	2.47E-07
	propane	2.76E-09	3.58E-12
	I-butane	7.44E-16	4.97E-24
	n-butane	1.02E-15	1.01E-23
	I-pentane	1.10E-22	5.40E-33
	n-pentane	4.87E-23	3.51E-33
	CO	1.12E-04	8.20E-02
	CO2	2.59E-02	2.17E-02
	hydrogen	3.36E-02	0.762706
	h20	0.54387	8.69E-02
	n2	9.56E-49	8.11E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	4.08E-25

S/C	R-101	Inlet	Outlet
3	methane	0.135817	3.41E-04
	ethane	5.16E-03	4.34E-03
	propane	3.14E-03	2.64E-03
	I-butane	6.96E-04	5.85E-04
	n-butane	6.10E-04	5.13E-04
	I-pentane	2.44E-04	2.05E-04
	n-pentane	1.77E-04	1.49E-04
	CO	6.44E-02	0.16254
	CO2	1.82E-02	2.09E-02
	hydrogen	0.599496	0.713173
	h20	8.96E-02	9.46E-02
	n2	6.38E-49	8.41E-49
	Carbon	0	1.00E-45
	oxygen	8.25E-02	8.41E-20

S/C	B-101	Inlet	Outlet
4	methane	0.396425	4.54E-02
	ethane	1.83E-05	2.27E-07
	propane	2.76E-09	3.09E-12
	I-butane	7.44E-16	3.30E-24
	n-butane	1.02E-15	6.72E-24
	I-pentane	1.10E-22	3.19E-33
	n-pentane	4.87E-23	2.07E-33
	CO	1.12E-04	6.94E-02
	CO2	2.59E-02	1.69E-02
	hydrogen	3.36E-02	0.785654
	h20	0.54387	8.26E-02
	n2	9.56E-49	8.44E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	3.50E-25

S/C	R-101	Inlet	Outlet
4	methane	0.125793	7.74E-04
	ethane	4.64E-03	3.95E-03
	propane	2.83E-03	2.40E-03
	I-butane	6.26E-04	5.32E-04
	n-butane	5.49E-04	4.67E-04
	I-pentane	2.19E-04	1.87E-04
	n-pentane	1.60E-04	1.36E-04
	CO	5.61E-02	0.147567
	CO2	1.47E-02	1.89E-02
	hydrogen	0.634373	0.738447
	h20	8.58E-02	8.67E-02
	n2	6.81E-49	8.51E-49
	Carbon	0	1.00E-45
	oxygen	7.42E-02	1.31E-20

S/C	B-101	Inlet	Outlet
5	methane	0.396425	4.42E-02
	ethane	1.83E-05	2.09E-07
	propane	2.76E-09	2.71E-12
	I-butane	7.44E-16	2.27E-24
	n-butane	1.02E-15	4.63E-24
	I-pentane	1.10E-22	1.98E-33
	n-pentane	4.87E-23	1.28E-33
	CO	1.12E-04	5.94E-02
	CO2	2.59E-02	1.35E-02
	hydrogen	3.36E-02	0.804011
	h20	0.54387	7.88E-02
	n2	9.56E-49	8.68E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	2.96E-25

S/C	R-101	Inlet	Outlet
5	methane	0.117476	1.50E-03
	ethane	4.22E-03	3.62E-03
	propane	2.57E-03	2.21E-03
	I-butane	5.69E-04	4.89E-04
	n-butane	4.99E-04	4.28E-04
	I-pentane	1.99E-04	1.71E-04
	n-pentane	1.45E-04	1.25E-04
	CO	4.90E-02	0.134838
	CO2	1.21E-02	1.71E-02
	hydrogen	0.663315	0.758979
	h20	8.24E-02	8.05E-02
	n2	7.17E-49	8.59E-49
	Carbon	0	1.00E-45
	oxygen	6.74E-02	2.85E-21

S/C	B-101	Inlet	Outlet
6	methane	0.396425	4.32E-02
	ethane	1.83E-05	1.94E-07
	propane	2.76E-09	2.40E-12
	I-butane	7.44E-16	1.61E-24
	n-butane	1.02E-15	3.28E-24
	I-pentane	1.10E-22	1.27E-33
	n-pentane	4.87E-23	8.24E-34
	CO	1.12E-04	5.13E-02
	CO2	2.59E-02	1.10E-02
	hydrogen	3.36E-02	0.819053
	h20	0.54387	7.54E-02
	n2	9.56E-49	8.88E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	2.48E-25

S/C	R-101	Inlet	Outlet
6	methane	0.110449	2.49E-03
	ethane	3.86E-03	3.35E-03
	propane	2.35E-03	2.04E-03
	I-butane	5.21E-04	4.52E-04
	n-butane	4.57E-04	3.96E-04
	I-pentane	1.83E-04	1.58E-04
	n-pentane	1.33E-04	1.15E-04
	CO	4.31E-02	0.123808
	CO2	1.01E-02	1.56E-02
	hydrogen	0.687727	0.775792
	h20	7.93E-02	7.58E-02
	n2	7.46E-49	8.67E-49
	Carbon	0	1.00E-45
	oxygen	6.18E-02	8.48E-22

S/C	B-101	Inlet	Outlet
7	methane	0.396425	4.22E-02
	ethane	1.83E-05	1.81E-07
	propane	2.76E-09	2.13E-12
	I-butane	7.44E-16	1.17E-24
	n-butane	1.02E-15	2.38E-24
	I-pentane	1.10E-22	8.41E-34
	n-pentane	4.87E-23	5.45E-34
	CO	1.12E-04	4.46E-02
	CO2	2.59E-02	9.12E-03
	hydrogen	3.36E-02	0.831615
	h20	0.54387	7.24E-02
	n2	9.56E-49	9.04E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	2.06E-25

S/C	R-101	Inlet	Outlet
7	methane	0.104425	3.66E-03
	ethane	3.56E-03	3.12E-03
	propane	2.17E-03	1.90E-03
	I-butane	4.81E-04	4.20E-04
	n-butane	4.21E-04	3.69E-04
	I-pentane	1.69E-04	1.47E-04
	n-pentane	1.23E-04	1.07E-04
	CO	3.80E-02	0.114121
	CO2	8.57E-03	1.43E-02
	hydrogen	0.708596	0.789753
	h20	7.65E-02	7.21E-02
	n2	7.71E-49	8.75E-49
	Carbon	0	1.00E-45
	oxygen	5.70E-02	3.27E-22

S/C	B-101	Inlet	Outlet
8	methane	0.396425	4.13E-02
	ethane	1.83E-05	1.70E-07
	propane	2.76E-09	1.91E-12
	I-butane	7.44E-16	8.63E-25
	n-butane	1.02E-15	1.75E-24
	I-pentane	1.10E-22	5.68E-34
	n-pentane	4.87E-23	3.67E-34
	CO	1.12E-04	3.90E-02
	CO2	2.59E-02	7.63E-03
	hydrogen	3.36E-02	0.842281
	h20	0.54387	6.98E-02
	n2	9.56E-49	9.18E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	1.71E-25

S/C	R-101	Inlet	Outlet
8	methane	9.92E-02	4.92E-03
	ethane	3.31E-03	2.92E-03
	propane	2.02E-03	1.78E-03
	I-butane	4.46E-04	3.93E-04
	n-butane	3.91E-04	3.45E-04
	I-pentane	1.56E-04	1.38E-04
	n-pentane	1.14E-04	1.00E-04
	CO	3.36E-02	0.10554
	CO2	7.32E-03	1.31E-02
	hydrogen	0.726648	0.801546
	h20	7.39E-02	6.92E-02
	n2	7.92E-49	8.82E-49
	Carbon	0	1.00E-45
	oxygen	5.29E-02	1.54E-22

S/C	B-101	Inlet	Outlet
9	methane	0.396425	4.05E-02
	ethane	1.83E-05	1.60E-07
	propane	2.76E-09	1.72E-12
	I-butane	7.44E-16	6.44E-25
	n-butane	1.02E-15	1.31E-24
	I-pentane	1.10E-22	3.90E-34
	n-pentane	4.87E-23	2.52E-34
	CO	1.12E-04	3.42E-02
	CO2	2.59E-02	6.44E-03
	hydrogen	3.36E-02	0.85146
	h20	0.54387	6.74E-02
	n2	9.56E-49	9.29E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	1.42E-25

S/C	R-101	Inlet	Outlet
9	methane	9.46E-02	6.18E-03
	ethane	3.09E-03	2.74E-03
	propane	1.88E-03	1.67E-03
	I-butane	4.16E-04	3.70E-04
	n-butane	3.65E-04	3.24E-04
	I-pentane	1.46E-04	1.30E-04
	n-pentane	1.06E-04	9.42E-05
	CO	2.98E-02	9.79E-02
	CO2	6.31E-03	1.20E-02
	hydrogen	0.742424	0.81168
	h20	7.15E-02	6.69E-02
	n2	8.10E-49	8.88E-49
	Carbon	0	1.00E-45
	oxygen	4.93E-02	8.32E-23

S/C	B-101	Inlet	Outlet
10	methane	0.396425	3.98E-02
	ethane	1.83E-05	1.50E-07
	propane	2.76E-09	1.56E-12
	I-butane	7.44E-16	4.86E-25
	n-butane	1.02E-15	9.83E-25
	I-pentane	1.10E-22	2.71E-34
	n-pentane	4.87E-23	1.75E-34
	CO	1.12E-04	3.01E-02
	CO2	2.59E-02	5.48E-03
	hydrogen	3.36E-02	0.859455
	h20	0.54387	6.52E-02
	n2	9.56E-49	9.38E-49
	Carbon	0	1.00E-45
	oxygen	9.56E-49	1.17E-25

S/C	R-101	Inlet	Outlet
10	methane	9.05E-02	7.40E-03
	ethane	2.89E-03	2.59E-03
	propane	1.76E-03	1.58E-03
	I-butane	3.90E-04	3.49E-04
	n-butane	3.42E-04	3.06E-04
	I-pentane	1.37E-04	1.22E-04
	n-pentane	9.94E-05	8.89E-05
	CO	2.65E-02	9.10E-02
	CO2	5.47E-03	1.11E-02
	hydrogen	0.756338	0.820516
	h20	6.93E-02	6.49E-02
	n2	8.26E-49	8.94E-49
	Carbon	0	1.00E-45
	oxygen	4.62E-02	5.00E-23

Appendix

Extracted data for reformer temperature analysis from HYSYS

Reactor corresponding temperature (^{o}C)

Steam	SMR	POX
400	574	935
450	577	946
500	580	957
550	583	967
600	586	978
650	590	989
700	593	1001
750	597	1012
800	601	1023

	B-101	Inlet	Outlet		R-101	Inlet	Outlet
400	methane	0.124955	2.88E-05		methane	1648.974	0.443099
	ethane	5.32E-03	4.57E-03		ethane	70.17073	70.17073
	propane	3.24E-03	2.78E-03		propane	42.75401	42.75401
	I-butane	7.17E-04	6.16E-04		I-butane	9.465822	9.465822
	n-butane	6.29E-04	5.40E-04		n-butane	8.296057	8.296057
	I-pentane	2.52E-04	2.16E-04		I-pentane	3.31932	3.31932
	n-pentane	1.83E-04	1.57E-04		n-pentane	2.412827	2.412827
	CO	8.34E-02	0.175133		CO	1100.5	2692.034
	CO2	1.69E-02	1.82E-02		CO2	223.3941	280.3911
	hydrogen	0.600251	0.69476		hydrogen	7921.203	10679.39
	h20	7.91E-02	0.102962		h20	1043.797	1582.67

450	methane	0.123087	2.36E-05
	ethane	5.30E-03	4.56E-03
	propane	3.23E-03	2.78E-03
	I-butane	7.15E-04	6.16E-04
	n-butane	6.27E-04	5.40E-04
	I-pentane	2.51E-04	2.16E-04
	n-pentane	1.82E-04	1.57E-04
	CO	8.50E-02	0.175547
	CO2	1.65E-02	1.78E-02
	hydrogen	0.602558	0.694358
	h20	7.77E-02	0.103366

methane	1629.182	0.362049
ethane	70.17059	70.17059
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1125.373	2698.418
CO2	218.313	274.088
hydrogen	7975.497	10673.33
h20	1029.086	1588.891

500	methane	0.121244	1.93E-05
	ethane	5.29E-03	4.56E-03
	propane	3.22E-03	2.78E-03
	I-butane	7.13E-04	6.16E-04
	n-butane	6.25E-04	5.40E-04
	I-pentane	2.50E-04	2.16E-04
	n-pentane	1.82E-04	1.57E-04
	CO	8.66E-02	0.175946
	CO2	1.61E-02	1.74E-02
	hydrogen	0.604823	0.693969
	h20	7.64E-02	0.103757

methane	1609.554	0.296529
ethane	70.17047	70.17047
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1150.168	2704.577
CO2	213.1472	267.9949
hydrogen	8029.217	10667.44
h20	1014.624	1594.919

550	methane	0.119426	1.58E-05
	ethane	5.27E-03	4.56E-03
	propane	3.21E-03	2.78E-03
	I-butane	7.11E-04	6.16E-04
	n-butane	6.23E-04	5.40E-04
	I-pentane	2.49E-04	2.16E-04
	n-pentane	1.81E-04	1.57E-04
	CO	8.82E-02	0.176332
	CO2	1.56E-02	1.71E-02
	hydrogen	0.607047	0.69359
	h20	7.51E-02	0.104137

methane	1590.076	0.243366
ethane	70.17035	70.17035
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1174.901	2710.53
CO2	207.8917	262.0957
hydrogen	8082.394	10661.7
h20	1000.402	1600.765

600	methane	0.117641	1.30E-05
	ethane	5.26E-03	4.56E-03
	propane	3.20E-03	2.78E-03
	I-butane	7.09E-04	6.16E-04
	n-butane	6.21E-04	5.40E-04
	I-pentane	2.49E-04	2.16E-04
	n-pentane	1.81E-04	1.57E-04
	CO	8.98E-02	0.176705
	CO2	1.52E-02	1.67E-02
	hydrogen	0.609222	0.693224
	h20	7.39E-02	0.104504

methane	1570.833	0.200217
ethane	70.17023	70.17023
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1199.469	2716.273
CO2	202.5662	256.3953
hydrogen	8134.798	10656.13
h20	986.4839	1606.422

650	methane	0.115885	1.07E-05
	ethane	5.24E-03	4.56E-03
	propane	3.19E-03	2.78E-03
	I-butane	7.07E-04	6.16E-04
	n-butane	6.20E-04	5.40E-04
	I-pentane	2.48E-04	2.16E-04
	n-pentane	1.80E-04	1.57E-04
	CO	9.14E-02	0.177065
	CO2	1.47E-02	1.63E-02
	hydrogen	0.61135	0.692869
	h20	7.27E-02	0.104861

methane	1551.799	0.165031
ethane	70.17013	70.17013
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1223.911	2721.831
CO2	197.1587	250.8731
hydrogen	8186.493	10650.71
h20	972.8571	1611.908

700	methane	0.114164	8.87E-06
	ethane	5.23E-03	4.56E-03
	propane	3.18E-03	2.78E-03
	I-butane	7.05E-04	6.16E-04
	n-butane	6.18E-04	5.40E-04
	I-pentane	2.47E-04	2.16E-04
	n-pentane	1.80E-04	1.57E-04
	CO	9.29E-02	0.177414
	CO2	1.43E-02	1.60E-02
	hydrogen	0.613426	0.692524
	h20	7.15E-02	0.105206

methane	1533.035	0.136298
ethane	70.17003	70.17003
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1248.156	2727.207
CO2	191.6786	245.5262
hydrogen	8237.307	10645.45
h20	959.5724	1617.226

750	methane	0.112484	7.34E-06
	ethane	5.21E-03	4.56E-03
	propane	3.18E-03	2.78E-03
	I-butane	7.03E-04	6.16E-04
	n-butane	6.16E-04	5.40E-04
	I-pentane	2.47E-04	2.16E-04
	n-pentane	1.79E-04	1.57E-04
	CO	9.45E-02	0.177752
	CO2	1.38E-02	1.56E-02
	hydrogen	0.61544	0.69219
	h20	7.03E-02	0.105541

methane	1514.615	0.112802
ethane	70.16993	70.16993
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1272.118	2732.404
CO2	186.1372	240.3526
hydrogen	8287.027	10640.35
h20	946.6935	1622.376

800	methane	0.110851	6.09E-06
	ethane	5.20E-03	4.56E-03
	propane	3.17E-03	2.78E-03
	I-butane	7.01E-04	6.16E-04
	n-butane	6.14E-04	5.40E-04
	I-pentane	2.46E-04	2.16E-04
	n-pentane	1.79E-04	1.57E-04
	CO	9.60E-02	0.178078
	CO2	1.34E-02	1.53E-02
	hydrogen	0.617384	0.691866
	h20	6.92E-02	0.105865

methane	1496.616	9.36E-02
ethane	70.16985	70.16985
propane	42.75401	42.75401
I-butane	9.465822	9.465822
n-butane	8.296057	8.296057
I-pentane	3.31932	3.31932
n-pentane	2.412827	2.412827
CO	1295.709	2737.428
CO2	180.5441	235.348
hydrogen	8335.428	10635.4
h20	934.2883	1627.361

Appendix

Sample worksheet of HYSYS simulation model

Petronas
Calgary, Alberta
CANADA

Case Name:	C:\Documents and Settings\Lau\My Documents\Final Year Project\Hys
Unit Set:	SI
Date/Time:	Sun Jan 11 03:02:09 2004

Gibbs Reactor: D-103

CONNECTIONS

Inlet Stream Connections

Stream Name	From Unit Operation	
1	Mixer	Mixer 1

Outlet Stream Connections

Stream Name	To Unit Operation	
03 outlet	Mixer:	Mixer 2
03 condensate		

Energy Stream Connections

Stream Name	From Unit Operation

PARAMETERS

Physical Parameters		Optional Heat Transfer: Heating	
Delta P	**Vessel Volume**	**Duty**	**Energy Stream**
0.0000 kPa *	15.00 m3 *	0.0000 kJ/h	

User Variables

REACTIONS OVERALL

REACTIONS SUMMARY: D-103

Name	% Conversion	Base Component	Equilibrium Constant	Rxn Extent (kgmole/h)	Est. Extent (kgmole/h)
ne reforming	—	Ethane	—	—	—
ane reforming	—	i-Butane	—	—	—
ntane reforming	—	i-Pentane	—	—	—
tane reforming	—	n-Butane	—	—	—
ntane reforming	—	n-Pentane	—	—	—
ane reforming	—	Propane	—	—	—
ane Reform	—	Methane	—	—	—

REACTOR COMPONENT SUMMARY

Components	Total Inflow (kgmole/h)	Total Reaction (kgmole/h)	Total Outflow (kgmole/h)	Gibbs Energy (kJ/kgmole)
ane	—	—	—	—
ne	—	—	—	—
ane	—	—	—	—
tane	—	—	—	—
tane	—	—	—	—
ntane	—	—	—	—
entane	—	—	—	—
	—	—	—	—
2	—	—	—	—
rogen	—	—	—	—
	—	—	—	—
gen	—	—	—	—
bon	—	—	—	—
gen	—	—	—	—

Gibbs Reactor: D-103 (continued)

REACTION DETAILS

MOLE FLOW SPECIFICATIONS

Components	Total Feed (kgmole/h)	Total Prod (kgmole/h)	Inerts	Frac Spec	Fixed Spec (kgmole/h)
Methane	1261	1510	No	---	---
Ethane	65.67	6.979e-002	No	---	---
Propane	36.14	1.052e-005	No	---	---
i-Butane	8.860	2.835e-012	No	---	---
n-Butane	7.765	3.898e-012	No	---	---
i-Pentane	3.106	4.178e-019	No	---	---
n-Pentane	2.259	1.855e-019	No	---	---
CO	0.0000	0.4271	No	---	---
CO2	14.77	98.78	No	---	---
Hydrogen	0.0000	128.1	No	---	---
H2O	2240	2072	No	---	---
Nitrogen	0.0000	0.0000	No	---	---
Carbon	0.0000	0.0000	No	---	---
Oxygen	0.0000	0.0000	No	---	---

ATOM MATRIX DATA

	C	H	O	N		
Methane	1.000 *	4.000 *	0.0000 *	0.0000 *		
Ethane	2.000 *	6.000 *	0.0000 *	0.0000 *		
Propane	3.000 *	8.000 *	0.0000 *	0.0000 *		
i-Butane	4.000 *	10.00 *	0.0000 *	0.0000 *		
n-Butane	4.000 *	10.00 *	0.0000 *	0.0000 *		
i-Pentane	5.000 *	12.00 *	0.0000 *	0.0000 *		
n-Pentane	5.000 *	12.00 *	0.0000 *	0.0000 *		
CO	1.000 *	0.0000 *	1.000 *	0.0000 *		
CO2	1.000 *	0.0000 *	2.000 *	0.0000 *		
Hydrogen	0.0000 *	2.000 *	0.0000 *	0.0000 *		
H2O	0.0000 *	2.000 *	1.000 *	0.0000 *		
Nitrogen	0.0000 *	0.0000 *	0.0000 *	2.000 *		
Carbon	1.000 *	0.0000 *	0.0000 *	0.0000 *		
Oxygen	0.0000 *	0.0000 *	2.000 *	0.0000 *		

PROPERTIES

feed

		Overall	Vapour Phase			
our/Phase Fraction		1.0000	1.0000			
perature:	(C)	395.2	395.2			
ssure:	(kPa)	4000	4000			
ar Flow	(kgmole/h)	3640	3640			
s Flow	(kg/h)	6.616e+004	6.616e+004			
id Volume Flow	(m3/h)	119.8	119.8			
ar Enthalpy	(kJ/kgmole)	-1.646e+005	-1.646e+005			
s Enthalpy	(kJ/kg)	-9054	-9054			
ar Entropy	(kJ/kgmole-C)	185.5	185.5			
s Entropy	(kJ/kg-C)	10.21	10.21			
t Flow	(kJ/h)	-5.991e+008	-5.991e+008			
ar Density	(kgmole/m3)	0.7329	0.7329			
s Density	(kg/m3)	13.32	13.32			
Liquid Mass Density	(kg/m3)	600.4	600.4			
ar Heat Capacity	(kJ/kgmole-C)	48.56	48.56			
s Heat Capacity	(kJ/kg-C)	2.672	2.672			

Gibbs Reactor: D-103 (continued)

PROPERTIES

feed

	Overall	Vapour Phase			
mal Conductivity (W/m-K)	7.198e-002	7.198e-002			
osity (cP)	2.091e-002	2.091e-002			
ace Tension (dyne/cm)	---	---			
cular Weight	18.18	18.18			
ctor	0.9822	0.9822			

D-103 condensate

	Overall	Vapour Phase	Liquid Phase	Aqueous Phase	
ur/Phase Fraction	0.0000	0.0000	0.5000	0.5000	
perature: (C)	385.8	385.8	385.8	385.8	
sure: (kPa)	4000	4000	4000	4000	
r Flow (kgmole/h)	0.0000	0.0000	0.0000	0.0000	
s Flow (kg/h)	0.0000	0.0000	0.0000	0.0000	
id Volume Flow (m3/h)	0.0000	0.0000	0.0000	0.0000	
r Enthalpy (kJ/kgmole)	-1.573e+005	-1.573e+005	-1.573e+005	-1.573e+005	
s Enthalpy (kJ/kg)	-9054	-9054	-9054	-9054	
r Entropy (kJ/kgmole-C)	182.8	182.8	182.8	182.8	
s Entropy (kJ/kg-C)	10.53	10.53	10.53	10.53	
Flow (kJ/h)	0.0000	0.0000	0.0000	0.0000	
r Density (kgmole/m3)	0.7399	0.7399	0.7399	0.7399	
s Density (kg/m3)	12.85	12.85	12.85	12.85	
iquid Mass Density (kg/m3)	526.1	526.1	526.1	526.1	
r Heat Capacity (kJ/kgmole-C)	45.99	45.99	45.99	45.99	
s Heat Capacity (kJ/kg-C)	2.648	2.648	2.648	2.648	
mal Conductivity (W/m-K)	0.1743	7.644e-002	0.1743	0.1743	
osity (cP)	3.341e-002	2.116e-002	5.523e-003	5.523e-003	
ace Tension (dyne/cm)	---	---	0.0000	0.0000	
cular Weight	17.37	17.37	17.37	17.37	
ctor	---	0.9868	0.9868	0.9868	

D-103 outlet

	Overall	Vapour Phase	Liquid Phase	Aqueous Phase	
ur/Phase Fraction	1.0000	1.0000	0.0000	0.0000	
perature: (C)	385.8	385.8	385.8	385.8	
sure: (kPa)	4000	4000	4000	4000	
r Flow (kgmole/h)	3809	3809	0.0000	0.0000	
s Flow (kg/h)	6.616e+004	6.616e+004	0.0000	0.0000	
id Volume Flow (m3/h)	127.3	127.3	0.0000	0.0000	
r Enthalpy (kJ/kgmole)	-1.573e+005	-1.573e+005	-1.573e+005	-1.573e+005	
s Enthalpy (kJ/kg)	-9054	-9054	-9054	-9054	
r Entropy (kJ/kgmole-C)	182.8	182.8	182.8	182.8	
s Entropy (kJ/kg-C)	10.53	10.53	10.53	10.53	
Flow (kJ/h)	-5.991e+008	-5.991e+008	0.0000	0.0000	
r Density (kgmole/m3)	0.7399	0.7399	0.7399	0.7399	
s Density (kg/m3)	12.85	12.85	12.85	12.85	
Liquid Mass Density (kg/m3)	526.1	526.1	526.1	526.1	
r Heat Capacity (kJ/kgmole-C)	45.99	45.99	45.99	45.99	
s Heat Capacity (kJ/kg-C)	2.648	2.648	2.648	2.648	
rmal Conductivity (W/m-K)	7.644e-002	7.644e-002	0.1743	0.1743	
osity (cP)	2.116e-002	2.116e-002	5.523e-003	5.523e-003	
ace Tension (dyne/cm)	---	---	0.0000	0.0000	
cular Weight	17.37	17.37	17.37	17.37	
ctor	0.9868	0.9868	0.9868	0.9868	

Gibbs Reactor: D-103 (continued)

DYNAMICS

Vessel Parameters: Initialize from Product

el Volume	(m3)	15.00 *	Level Calculator		Vertical cylinder
el Diameter	(m)	2.335	Fraction Calculator		Use levels and nozzles
el Height	(m)	3.503	Feed Delta P	(kPa)	0.0000 *
d Level Percent	(%)	50.00	Vessel Pressure	(kPa)	4000

Holdup: Vessel Levels

Phase	Level (m)	Percent (%)	Volume (m3)
Vapour	---	---	0.0000
Liquid	---	---	0.0000
Aqueous	---	---	0.0000

Holdup: Details

Phase	Accumulation (kgmole/h)	Moles (kgmole)	Volume (m3)
Vapour	0.0000	0.0000 *	0.0000
Liquid	0.0000	0.0000 *	0.0000
Aqueous	0.0000	0.0000 *	0.0000
Total	**0.0000**	**0.0000**	**0.0000**

Petronas
Calgary, Alberta
CANADA

Case Name:	C:\Documents and Settings\Lau\My Documents\Final Year Project\Hys
Unit Set:	SI
Date/Time:	Sun Jan 11 03:13:49 2004

Gibbs Reactor: B-101

CONNECTIONS

Inlet Stream Connections

Stream Name	From Unit Operation	
01 feed	Mixer	Mixer 2

Outlet Stream Connections

Stream Name	To Unit Operation	
01 outlet	Mixer:	Mixer 3
01 condensate		

Energy Stream Connections

Stream Name	From Unit Operation
t	

PARAMETERS

Physical Parameters		Optional Heat Transfer: Heating	
Delta P	**Vessel Volume**	**Duty**	**Energy Stream**
0.0000 kPa *	22.50 m3 *	3.500e+008 kJ/h *	Heat

User Variables

REACTIONS OVERALL

REACTIONS SUMMARY: Steam Reforming

Name	% Conversion	Base Component	Equilibrium Constant	Rxn Extent (kgmole/h)	Est. Extent (kgmole/h)
1	---	CO	---	---	---
2	---	CO	---	---	---
3	---	Methane	---	---	---
ne reforming	---	Ethane	---	---	---
ane reforming	---	i-Butane	---	---	---
tane reforming	---	i-Pentane	---	---	---
tane reforming	---	n-Butane	---	---	---
ntane reforming	---	n-Pentane	---	---	---
ane reforming	---	Propane	---	---	---
ane Reform	---	Methane	---	---	---

REACTOR COMPONENT SUMMARY

Components	Total Inflow (kgmole/h)	Total Reaction (kgmole/h)	Total Outflow (kgmole/h)	Gibbs Energy (kJ/kgmole)
ane	---	---	---	---
ne	---	---	---	---
ane	---	---	---	---
tane	---	---	---	---
tane	---	---	---	---
ntane	---	---	---	---
ntane	---	---	---	---
	---	---	---	---
	---	---	---	---
rogen	---	---	---	---
	---	---	---	---
gen	---	---	---	---
on	---	---	---	---
gen	---	---	---	---

Gibbs Reactor: B-101 (continued)

REACTION DETAILS

MOLE FLOW SPECIFICATIONS

Components	Total Feed (kgmole/h)	Total Prod (kgmole/h)	Inerts	Frac Spec	Fixed Spec (kgmole/h)
Methane	1510	937.7	No	---	---
Ethane	6.979e-002	6.795e-002	No	---	---
Propane	1.052e-005	1.482e-005	No	---	---
i-Butane	2.835e-012	9.544e-013	No	---	---
n-Butane	3.898e-012	2.529e-012	No	---	---
i-Pentane	4.178e-019	1.997e-019	No	---	---
n-Pentane	1.855e-019	1.663e-019	No	---	---
CO	0.4271	597.3	No	---	---
CO2	98.78	74.09	No	---	---
Hydrogen	6620	8312	No	---	---
H2O	2072	1524	No	---	---
Nitrogen	3.640e-045	0.0000	No	---	---
Carbon	0.0000	0.0000	No	---	---
Oxygen	3.640e-045	3.047e-015	No	---	---

ATOM MATRIX DATA

	C	H	O	N		
Methane	1.000 *	4.000 *	0.0000 *	0.0000 *		
Ethane	2.000 *	6.000 *	0.0000 *	0.0000 *		
Propane	3.000 *	8.000 *	0.0000 *	0.0000 *		
i-Butane	4.000 *	10.00 *	0.0000 *	0.0000 *		
n-Butane	4.000 *	10.00 *	0.0000 *	0.0000 *		
i-Pentane	5.000 *	12.00 *	0.0000 *	0.0000 *		
n-Pentane	5.000 *	12.00 *	0.0000 *	0.0000 *		
CO	1.000 *	0.0000 *	1.000 *	0.0000 *		
CO2	1.000 *	0.0000 *	2.000 *	0.0000 *		
Hydrogen	0.0000 *	2.000 *	0.0000 *	0.0000 *		
H2O	0.0000 *	2.000 *	1.000 *	0.0000 *		
Nitrogen	0.0000 *	0.0000 *	0.0000 *	2.000 *		
Carbon	1.000 *	0.0000 *	0.0000 *	0.0000 *		
Oxygen	0.0000 *	0.0000 *	2.000 *	0.0000 *		

PROPERTIES

B-101 feed

	Overall	Vapour Phase			
our/Phase Fraction	1.0000	1.0000			
perature: (C)	391.8	391.8			
sure: (kPa)	4000	4000			
r Flow (kgmole/h)	1.030e+004	1.030e+004			
s Flow (kg/h)	7.925e+004	7.925e+004			
id Volume Flow (m3/h)	314.6	314.6			
r Enthalpy (kJ/kgmole)	-5.128e+004	-5.128e+004			
s Enthalpy (kJ/kg)	-6665	-6665			
r Entropy (kJ/kgmole-C)	145.6	145.6			
s Entropy (kJ/kg-C)	18.93	18.93			
Flow (kJ/h)	-5.282e+008	-5.282e+008			
r Density (kgmole/m3)	0.7192	0.7192			
s Density (kg/m3)	5.533	5.533			
Liquid Mass Density (kg/m3)	---	---			
r Heat Capacity (kJ/kgmole-C)	35.52	35.52			
s Heat Capacity (kJ/kg-C)	4.617	4.617			

Gibbs Reactor: B-101 (continued)

PROPERTIES

B-101 feed

	Overall	Vapour Phase			
mal Conductivity (W/m-K)	0.1864	0.1864			
osity (cP)	1.858e-002	1.858e-002			
ace Tension (dyne/cm)	—	—			
cular Weight	7.693	7.693			
ctor	1.006	1.006			

B-101 condensate

	Overall	Vapour Phase	Liquid Phase	Aqueous Phase	
our/Phase Fraction	0.0000	0.0000	0.5000	0.5000	
perature: (C)	946.5	946.5	946.5	946.5	
sure: (kPa)	4000	4000	4000	4000	
r Flow (kgmole/h)	0.0000	0.0000	0.0000	0.0000	
s Flow (kg/h)	0.0000	0.0000	0.0000	0.0000	
id Volume Flow (m3/h)	0.0000	0.0000	0.0000	0.0000	
r Enthalpy (kJ/kgmole)	-1.557e+004	-1.557e+004	-1.557e+004	-1.557e+004	
s Enthalpy (kJ/kg)	-2249	-2249	-2249	-2249	
r Entropy (kJ/kgmole-C)	159.8	159.8	159.8	159.8	
s Entropy (kJ/kg-C)	23.08	23.08	23.08	23.08	
t Flow (kJ/h)	0.0000	0.0000	0.0000	0.0000	
r Density (kgmole/m3)	0.3925	0.3925	0.3925	0.3925	
s Density (kg/m3)	2.718	2.718	2.718	2.718	
Liquid Mass Density (kg/m3)	—	—	—	—	
r Heat Capacity (kJ/kgmole-C)	37.18	37.18	37.18	37.18	
s Heat Capacity (kJ/kg-C)	5.369	5.369	5.369	5.369	
mal Conductivity (W/m-K)	4.167e-002	0.3278	4.167e-002	4.167e-002	
osity (cP)	1.707e-002	3.155e-002	2.821e-003	2.821e-003	
ace Tension (dyne/cm)	—	—	0.0000	0.0000	
cular Weight	6.924	6.924	6.924	6.924	
ctor	—	1.005	1.005	1.005	

B-101 outlet

	Overall	Vapour Phase	Liquid Phase	Aqueous Phase	
our/Phase Fraction	1.0000	1.0000	0.0000	0.0000	
perature: (C)	946.5	946.5	946.5	946.5	
sure: (kPa)	4000	4000	4000	4000	
r Flow (kgmole/h)	1.145e+004	1.145e+004	0.0000	0.0000	
s Flow (kg/h)	7.925e+004	7.925e+004	0.0000	0.0000	
id Volume Flow (m3/h)	342.5	342.5	0.0000	0.0000	
r Enthalpy (kJ/kgmole)	-1.557e+004	-1.557e+004	-1.557e+004	-1.557e+004	
s Enthalpy (kJ/kg)	-2249	-2249	-2249	-2249	
r Entropy (kJ/kgmole-C)	159.8	159.8	159.8	159.8	
s Entropy (kJ/kg-C)	23.08	23.08	23.08	23.08	
t Flow (kJ/h)	-1.782e+008	-1.782e+008	0.0000	0.0000	
r Density (kgmole/m3)	0.3925	0.3925	0.3925	0.3925	
s Density (kg/m3)	2.718	2.718	2.718	2.718	
Liquid Mass Density (kg/m3)	—	—	—	—	
r Heat Capacity (kJ/kgmole-C)	37.18	37.18	37.18	37.18	
s Heat Capacity (kJ/kg-C)	5.369	5.369	5.369	5.369	
mal Conductivity (W/m-K)	0.3278	0.3278	4.167e-002	4.167e-002	
osity (cP)	3.155e-002	3.155e-002	2.821e-003	2.821e-003	
ace Tension (dyne/cm)	—	—	0.0000	0.0000	
cular Weight	6.924	6.924	6.924	6.924	
ctor	1.005	1.005	1.005	1.005	

Gibbs Reactor: B-101 (continued)

DYNAMICS

Vessel Parameters: Initialize from Product

sel Volume	(m3)	22.50 *	Level Calculator		Vertical cylinder
sel Diameter	(m)	2.673	Fraction Calculator		Use levels and nozzles
sel Height	(m)	4.010	Feed Delta P	(kPa)	0.0000 *
id Level Percent	(%)	50.00	Vessel Pressure	(kPa)	4000

Holdup: Vessel Levels

Phase	Level (m)	Percent (%)	Volume (m3)
Vapour	---	---	0.0000
Liquid	---	---	0.0000
Aqueous	---	---	0.0000

Holdup: Details

Phase	Accumulation (kgmole/h)	Moles (kgmole)	Volume (m3)
Vapour	0.0000	0.0000 *	0.0000
Liquid	0.0000	0.0000 *	0.0000
Aqueous	0.0000	0.0000 *	0.0000
Total	**0.0000**	**0.0000**	**0.0000**

Liquid Heater Height as % of Vessel Volume

Top of Heater :	5.00 % *	Bottom of Heater :	0.00 % *

Heat Flow into the PFR: Heating

Gibbs Reactor: R-101

CONNECTIONS

Inlet Stream Connections

Stream Name	From Unit Operation	
01 feed	Mixer	Mixer 3

Outlet Stream Connections

Stream Name	To Unit Operation
01 outlet	
01 condensate	

Energy Stream Connections

Stream Name	From Unit Operation

PARAMETERS

Physical Parameters		Optional Heat Transfer: Heating	
Delta P	**Vessel Volume**	**Duty**	**Energy Stream**
5.000 kPa *	140.0 m3 *	0.0000 kJ/h	

User Variables

REACTIONS OVERALL

REACTIONS SUMMARY: R-101 set

Name	% Conversion	Base Component	Equilibrium Constant	Rxn Extent (kgmole/h)	Est. Extent (kgmole/h)
	—	Methane	—	—	—
	—	Methane	—	—	—
a+shift	—	Methane	—	—	—

REACTOR COMPONENT SUMMARY

Components	Total Inflow (kgmole/h)	Total Reaction (kgmole/h)	Total Outflow (kgmole/h)	Gibbs Energy (kJ/kgmole)
ane	—	—	—	—
ne	—	—	—	—
ane	—	—	—	—
tane	—	—	—	—
tane	—	—	—	—
ntane	—	—	—	—
entane	—	—	—	—
	—	—	—	—
2	—	—	—	—
rogen	—	—	—	—
	—	—	—	—
gen	—	—	—	—
on	—	—	—	—
gen	—	—	—	—

REACTION DETAILS

MOLE FLOW SPECIFICATIONS

Components	Total Feed (kgmole/h)	Total Prod (kgmole/h)	Inerts	Frac Spec	Fixed Spec (kgmole/h)
Methane	2286	513.5	No	—	—
Ethane	70.24	70.24	No	—	—
Propane	42.75	42.75	No	—	—
i-Butane	9.466	9.466	No	—	—
n-Butane	8.296	8.296	No	—	—
i-Pentane	3.319	3.319	No	—	—
n-Pentane	2.413	2.413	No	—	—
CO	597.3	2171	No	—	—
CO2	89.87	288.4	No	—	—

Gibbs Reactor: R-101 (continued)

REACTION DETAILS

MOLE FLOW SPECIFICATIONS

Components	Total Feed (kgmole/h)	Total Prod (kgmole/h)	Inerts	Frac Spec	Fixed Spec (kgmole/h)
Hydrogen	8312	1.158e+004	No	---	---
H2O	2524	2798	No	---	---
Nitrogen	1.030e-044	0.0000	No	---	---
Carbon	0.0000	0.0000	No	---	---
Oxygen	1122	1.859e-013	No	---	---

ATOM MATRIX DATA

	C	H	O	N		
Methane	1.000 *	4.000 *	0.0000 *	0.0000 *		
Ethane	2.000 *	6.000 *	0.0000 *	0.0000 *		
Propane	3.000 *	8.000 *	0.0000 *	0.0000 *		
i-Butane	4.000 *	10.00 *	0.0000 *	0.0000 *		
n-Butane	4.000 *	10.00 *	0.0000 *	0.0000 *		
i-Pentane	5.000 *	12.00 *	0.0000 *	0.0000 *		
n-Pentane	5.000 *	12.00 *	0.0000 *	0.0000 *		
CO	1.000 *	0.0000 *	1.000 *	0.0000 *		
CO2	1.000 *	0.0000 *	2.000 *	0.0000 *		
Hydrogen	0.0000 *	2.000 *	0.0000 *	0.0000 *		
H2O	0.0000 *	2.000 *	1.000 *	0.0000 *		
Nitrogen	0.0000 *	0.0000 *	0.0000 *	2.000 *		
Carbon	1.000 *	0.0000 *	0.0000 *	0.0000 *		
Oxygen	0.0000 *	0.0000 *	2.000 *	0.0000 *		

PROPERTIES

R-101 feed

	Overall	Vapour Phase			
ur/Phase Fraction	1.0000	1.0000			
erature: (C)	772.4	772.4			
sure: (kPa)	4000	4000			
Flow (kgmole/h)	1.507e+004	1.507e+004			
Flow (kg/h)	1.609e+005	1.609e+005			
Volume Flow (m3/h)	477.3	477.3			
Enthalpy (kJ/kgmole)	-3.242e+004	-3.242e+004			
Enthalpy (kJ/kg)	-3035	-3035			
Entropy (kJ/kgmole-C)	170.2	170.2			
Entropy (kJ/kg-C)	15.93	15.93			
Flow (kJ/h)	-4.884e+008	-4.884e+008			
Density (kgmole/m3)	0.4572	0.4572			
Density (kg/m3)	4.884	4.884			
iquid Mass Density (kg/m3)	---	---			
Heat Capacity (kJ/kgmole-C)	40.94	40.94			
Heat Capacity (kJ/kg-C)	3.833	3.833			
nal Conductivity (W/m-K)	0.2287	0.2287			
sity (cP)	3.043e-002	3.043e-002			
ce Tension (dyne/cm)	---	---			
ular Weight	10.68	10.68			
tor	1.006	1.006			

R-101 condensate

	Overall	Vapour Phase	Liquid Phase	Aqueous Phase	
ur/Phase Fraction	0.0000	0.0000	0.5000	0.5000	
erature: (C)	1030	1030	1030	1030	
sure: (kPa)	3995	3995	3995	3995	
Flow (kgmole/h)	0.0000	0.0000	0.0000	0.0000	
Flow (kg/h)	0.0000	0.0000	0.0000	0.0000	
Volume Flow (m3/h)	0.0000	0.0000	0.0000	0.0000	
Enthalpy (kJ/kgmole)	-2.793e+004	-2.793e+004	-2.793e+004	-2.793e+004	

Gibbs Reactor: R-101 (continued)

PROPERTIES

R-101 condensate

		Overall	Vapour Phase	Liquid Phase	Aqueous Phase
s Enthalpy	(kJ/kg)	-3035	-3035	-3035	-3035
ır Entropy	(kJ/kgmole-C)	165.0	165.0	165.0	165.0
s Entropy	(kJ/kg-C)	17.94	17.94	17.94	17.94
: Flow	(kJ/h)	0.0000	0.0000	0.0000	0.0000
ır Density	(kgmole/m3)	0.3671	0.3671	0.3671	0.3671
s Density	(kg/m3)	3.378	3.378	3.378	3.378
Liquid Mass Density	(kg/m3)	---	---	---	---
ır Heat Capacity	(kJ/kgmole-C)	37.07	37.07	37.07	37.07
s Heat Capacity	(kJ/kg-C)	4.029	4.029	4.029	4.029
mal Conductivity	(W/m-K)	4.578e-002	0.2978	4.578e-002	4.578e-002
osity	(cP)	1.915e-002	3.583e-002	3.166e-003	3.166e-003
ace Tension	(dyne/cm)	---	---	0.0000	0.0000
cular Weight		9.202	9.202	9.202	9.202
ctor		---	1.005	1.005	1.005

R-101 outlet

		Overall	Vapour Phase	Liquid Phase	Aqueous Phase
our/Phase Fraction		1.0000	1.0000	0.0000	0.0000
perature:	(C)	1030	1030	1030	1030
sure:	(kPa)	3995	3995	3995	3995
ır Flow	(kgmole/h)	1.749e+004	1.749e+004	0.0000	0.0000
s Flow	(kg/h)	1.609e+005	1.609e+005	0.0000	0.0000
id Volume Flow	(m3/h)	515.8	515.8	0.0000	0.0000
ır Enthalpy	(kJ/kgmole)	-2.793e+004	-2.793e+004	-2.793e+004	-2.793e+004
s Enthalpy	(kJ/kg)	-3035	-3035	-3035	-3035
ır Entropy	(kJ/kgmole-C)	165.0	165.0	165.0	165.0
s Entropy	(kJ/kg-C)	17.94	17.94	17.94	17.94
: Flow	(kJ/h)	-4.884e+008	-4.884e+008	0.0000	0.0000
ır Density	(kgmole/m3)	0.3671	0.3671	0.3671	0.3671
s Density	(kg/m3)	3.378	3.378	3.378	3.378
Liquid Mass Density	(kg/m3)	---	---	---	---
ır Heat Capacity	(kJ/kgmole-C)	37.07	37.07	37.07	37.07
s Heat Capacity	(kJ/kg-C)	4.029	4.029	4.029	4.029
mal Conductivity	(W/m-K)	0.2978	0.2978	4.578e-002	4.578e-002
osity	(cP)	3.583e-002	3.583e-002	3.166e-003	3.166e-003
ace Tension	(dyne/cm)	---	---	0.0000	0.0000
cular Weight		9.202	9.202	9.202	9.202
ctor		1.005	1.005	1.005	1.005

DYNAMICS

Vessel Paramters: Dry Start Up

sel Volume	(m3)	140.0 *	Level Calculator		Vertical cylinder
sel Diameter	(m)	4.916	Fraction Calculator		Use levels and nozzles
sel Height	(m)	7.375	Feed Delta P	(kPa)	5.000 *
id Level Percent	(%)	50.00	Vessel Pressure	(kPa)	3995

Holdup: Vessel Levels

Phase	Level (m)	Percent (%)	Volume (m3)
Vapour	---	---	0.0000
Liquid	---	---	0.0000
Aqueous	---	---	0.0000

Holdup: Details

Phase	Accumulation (kgmole/h)	Moles (kgmole)	Volume (m3)
Vapour	0.0000	0.0000 *	0.0000
Liquid	0.0000	0.0000 *	0.0000

Gibbs Reactor: R-101 (continued)

Phase	Accumulation (kgmole/h)	Moles (kgmole)	Volume (m3)
Aqueous	0.0000	0.0000 *	0.0000
Total	**0.0000**	**0.0000**	**0.0000**