



2011 National Student Design Competition



If there are any questions about the Design Competition, student chapter advisors and design course instructors are asked to contact:

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**Please read the rules on the following pages carefully
before submitting a solution to AIChE.**



October 2010

Dear Chemical Engineering Department Heads and Student Chapter Advisors,

I am pleased to send you the 2011 AIChE National Student Design Competition statement. Please forward it to those faculty teaching design courses. Following is this year's challenge:

“Gas to Liquids (GTL)”

As always, the names of the sponsoring organization and the authors are being withheld to ensure confidentiality. Both will be announced after the deadline- **Friday, June 3, 2011.**

- ❖ **An entry form is required for each participant** -- is available as a separate attachment, and must be submitted along with the completed solution.

We welcome participation by individuals and teams of up to three students. Please indicate the names of all team members on each entry form, and be advised that each team member is required to submit a separate entry form.

- ❖ **AIChE Student Membership Required** - Because the National Student Design Competition is a benefit of AIChE student membership, entrants must be AIChE national student members. Any non-member submissions will not be considered. To join, students can download a membership application form at <http://www.aiche.org/students/>.
- ❖ **All submissions must be submitted in an electronic format via postal mail on a CD.** Solutions must be submitted on a CD by postal mail or ground delivery -- postmarked no later than **Friday, June 3, 2011.** Please maintain a copy for your files.
- ❖ **Submissions must be no more than two documents (PDF or MS-Word formats only)** --totaling 100 or fewer pages of main text, with an allowable 100 pages of supplementary materials – in one of the following formats: PDF or MS-Word. The requested format is a single PDF file—the Adobe Acrobat program can be used to combine pages from different sources into one document.

Student Chapter Advisors are asked to select the best solution or solutions, not to exceed two from each category (individual and team).

Please take time to review the rules, found on the following pages. It is important that all solutions strictly adhere to the Final Report Format.

If I can be of assistance, please contact me at (646) 495-1333 or via email at studentchapters@aiche.org. Questions relating to the substance of the design problem should be directed to: Professor Richard L. Long, New Mexico State University, at (505) 646-2503 or riling@nmsu.edu.

Thank you for your support of this important student competition.

Sincerely,
June Lee



2011 AIChE National Student Design Competition

Contest Rules

Solutions will be graded on (a) substantial correctness of results and soundness of conclusions, (b) ingenuity and logic employed, (c) accuracy of computations, and (d) form of presentation.

Accuracy of computations is intended to mean primarily freedom from mistakes; extreme precision is not necessary.

It is to be assumed that the statement of the problem contains all the pertinent data except for those available in handbooks and literature references. The use of textbooks, handbooks, journal articles, and lecture notes is permitted.

Students may use any available commercial or library computer programs in preparing their solutions. Students are warned, however, that physical property data built into such programs may differ from data given in the problem statement. In such cases, as with data from literature sources, values given in the problem statement are most applicable. Students using commercial or library computer programs or other solution aids should so state in their reports and include proper references and documentation. Judging, however, will be based on the overall suitability of the solutions, not on skills in manipulating computer programs.

Departments, including advisors, faculty, or any other instructor, cannot provide technical aid specifically directed at the solution of the national student design competition.

The 2011 National Student Design Competition is designed to be solved either by an individual chemical engineering student working entirely alone, or a group of no more than three students working together. Solutions will be judged in two categories: individual and team. There are, however, other academically sound approaches to using the problem, and it is expected that some Advisors will use the problem as classroom material. The following confidentiality rules therefore apply:

1. For individual students or teams whose solutions may be considered for the contest: The problem may not be discussed with anyone (students, faculty, or others, in or out of class) before or during the period allowed for solutions. Discussion with faculty and students at that college or university is permitted only after complete final reports have been submitted to the Chapter Advisor.

2. For students whose solutions are not intended for the contest: Discussion with faculty and with other students at that college or university who are not participating in the contest is permitted.

3. For all students: The problem may not be discussed with students or faculty from other colleges and universities, or with individuals in the same institution who are still working on the problem for the contest, until after June 4, 2010. This is particularly important in cases where neighboring institutions may be using different schedules.



Submission of a solution for the competition implies strict adherence to the following conditions: **(Failure to comply will result in solutions being returned to the appropriate Faculty Advisor for revision. Revised submissions must meet the original deadline.)**

ELIGIBILITY

- ❖ ONLY AIChE NATIONAL STUDENT MEMBERS MAY SUBMIT A SOLUTION. Non-member entries will not be considered. To become a National Student member, you can join online at: <http://www.aiche.org/students/>.
- ❖ Entries must be submitted either by individuals or by teams of no more than three students. Each team member must meet all eligibility requirements.
- ❖ Each Faculty Advisor should select the best solution or solutions, not to exceed two from each category (individual and team), from his or her chapter and submit them per the instructions below.

TIMELINE FOR COMPLETING THE SOLUTION

- ❖ A period of no more than thirty (30) days is allowed for completion of the solution. This period may be selected at the discretion of the individual advisor, but in order to be eligible for an award, a solution must be postmarked no later than midnight June 4, 2010.
- ❖ The finished report should be submitted to the faculty advisor within the 30-day period.

REPORT FORMAT

- ❖ The body of the report must be suitable for reproduction, that is, computer-generated and in a printable format. Tables, supporting calculations and other appendix material may be handwritten.
- ❖ The solution itself must bear no reference to the students' names and institution by which it might be identified. Please expunge all such references to the degree possible.
- ❖ **Final submission of solutions to AIChE must be in electronic format (PDF or MS-Word).** The main text must be 100 pages or less, and an additional 100 page or less is allowable for supplementary material. The final submission to AIChE must consist of 1 or 2 electronic files.

SENDING THE SOLUTION TO AIChE

- ❖ There should not be any variation in form or content between the solution submitted to the Faculty Advisor and that sent to AIChE National. The Student Chapter Advisor, or Faculty Advisor, sponsoring the student(s), is asked to maintain the original manuscript(s).
- ❖ **Copy the electronic file (PDF or MS-Word) to a CD, accompanied by its corresponding entry form, and mail the CD to:**

**AIChE Awards Administrator
3 Park Avenue, 19th Floor
New York, NY 10016**

- ❖ **DEADLINE: Entries must be postmarked by Friday, June 3, 2011.**

2011 National Student Design Competition:
Gas to Liquids (GTL)

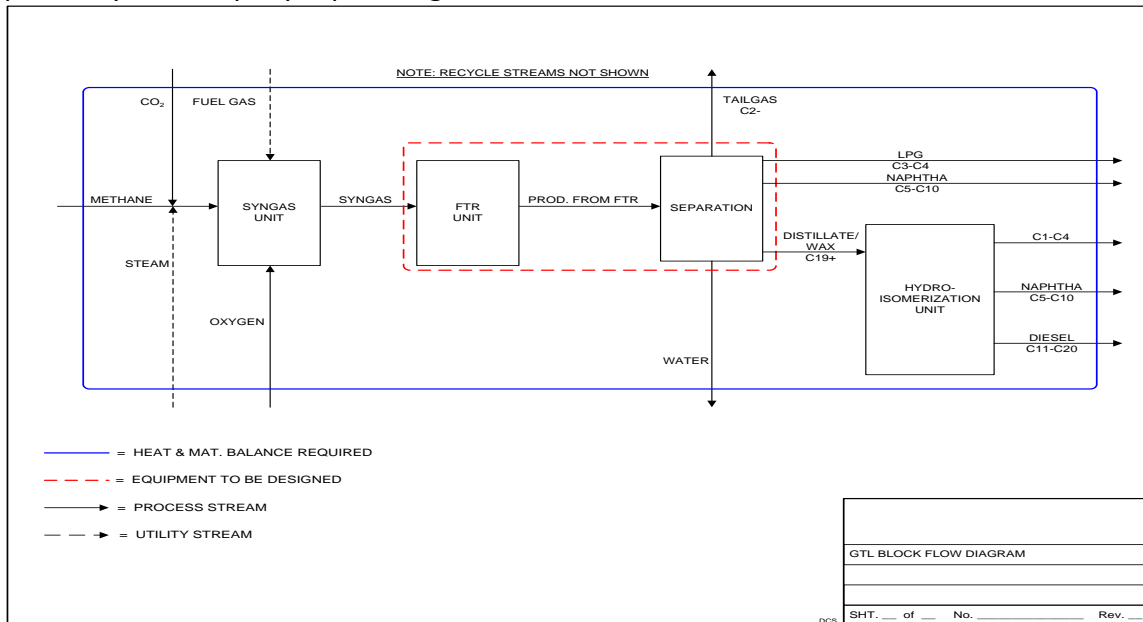
Introduction

The conversion of syngas (CO & H₂) to hydrocarbons using the Fischer-Tropsch synthesis is a proven method for the production of liquid fuels. Industrial fuel production using syngas and Fischer-Tropsch synthesis has been a viable option since the early 20th century, especially if petroleum reserves were unavailable or natural gas and/or coal reserves were abundant. Generation of syngas is possible with an array of carbon sources - coal, biomass, methane, etc. There are operating Gas to Liquids (GTL) processing facilities worldwide that convert the methane from natural gas to liquid fuel via syngas generation and Fischer-Tropsch synthesis(3).

As a Process Design Engineer you have been instructed by your company to provide the preliminary design package for a grass-roots Fischer-Tropsch Reaction unit (FTR), including reactor effluent separation facilities, as part of a planned GTL plant. Your company has specifically requested that you design a safe, environmentally clean, thermally integrated FTR with efficient capital and operating cost utilization. In addition, your company expects the FTR to effectively integrate with the other required units within the GTL plant to allow for the economically optimum diesel (C11-C20) and naphtha (C5-10, a feedstock for gasoline and chemicals) production.

Project Background

Your company is considering a GTL plant as an effective option to bring to market newly discovered gas deposits in a remote location. The company has the completed designs for a Syngas Unit (SU) and Hydro-Isomerization Unit (HI). A simplified diagram of the GTL process your company is planning is:



Although your company is not asking you to design any equipment for the SU and HI, they envision your design for the FTR as an opportunity to improve on the energy efficiency and operating expenses for the GTL plant as a whole.

Design Objectives

You must address and adhere to these specific objectives in the design package:

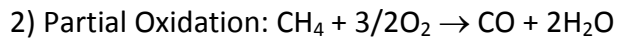
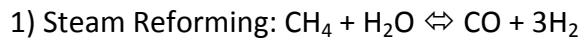
- 1) Safety/Environmental – Design must not pose any environmental, health or safety hazards that should have been mitigated with better equipment, instrumentation or control. Additionally, no continuous flaring/venting of hydrocarbons is permitted in the design – if necessary, hydrocarbons can be reused in the process.
- 2) Energy Efficiency & Lowest Environmental Impact – Defined as: (mass of carbon in finished products/mass of carbon in methane feed) x 100%. Finished products = LPG + Naphtha + Diesel. Other than safety and environmental performance, energy efficiency is next most important attribute that will determine acceptance of your design by your company.
- 3) Optimum Finished Liquid Fuel Production – Appropriate cost/benefit balance is achieved.
- 4) Economic Analysis (Discounted Cash Flow Rate of Return) - Economic analysis should reflect not only the designed equipment capital investment and expense costs, but also the expense costs of the Syngas, Air Separation Plant and Hydro-Isomerization Unit. In addition, specified capital recovery costs for both the Syngas and Hydro-Isomerization units (see page 10) will need to be added to the estimated total yearly expense costs. For economic calculations assume:
 - a. Project Life of 15 years
 - b. 15 year Straight Line Depreciation
 - c. 33% Tax Rate
 - d. Projected 3% yearly inflation
 - e. Total capital investment can be estimated by multiplying the equipment cost by 4.8. Multiplier will account for all associated direct costs, indirect costs and working capital.
 - f. Total yearly operating expenses above and beyond utilities can be estimated using 3% of the total capital investment. This estimate will cover fixed charges such as plant overhead costs, administrative costs, distribution & marketing and research & development
 - g. FTR Unit will have a 1 month turnaround to coincide w/ catalyst replacement
 - h. You may use equipment cost data from textbooks and other public sources

- 5) Feasible Design – Even though you are not providing the final design, your preliminary design should be viable as specified.
- 6) Realistic and Adequate Process Control – Control valves, instrumentation, analyzers, etc. on required equipment to provide safety and minimize personnel. It is not necessary to specify each component in detail; simply identify what they are and where in the process they are required.

Designed/Available Facilities

Syngas Unit

The SU will be immediately upstream of the FTR. The SU is being designed to convert the 500 MSCF/D (Actual Conditions: 500 PSIG, 100F) of clean methane to syngas. The heat required to drive the endothermic autothermal reforming reaction is supplied in-situ by partial oxidation of methane. Steam and CO₂ are required as feeds to drive the reforming reaction to make the desired molar ratio of H₂/CO. In the SU, three primary reactions occur (1):



The partial oxidation reaction runs to completion; the other two reactions run to equilibrium. The heat balance determines the amount of oxygen supplied. You may assume zero heat losses for the reactor.

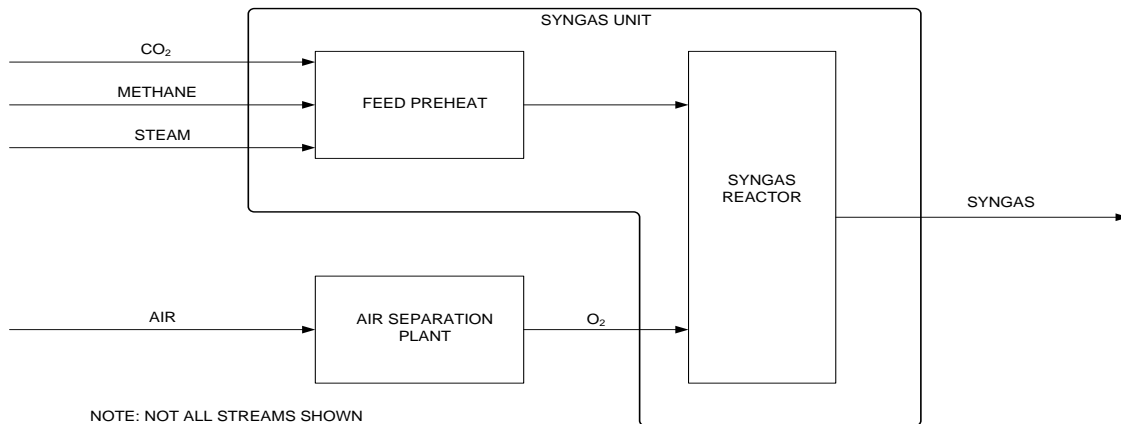
These reactions in combination determine the composition of the product gas from the reformer. Operating pressure, temperature, and feed composition will set the overall composition of the synthesis gas. You should consider the following ranges for reformer operating conditions:

- Temperature: 1600 - 1950°F
- Pressure: 300 - 500 PSIG
- Steam/CH₄ in Feed: 0.5 mol/mol minimum to prevent coking in feed preheater

You should target to make syngas with a H₂/CO molar ratio equal to the consumption ratio in the FTR (2:1). You will likely find that this requires supplemental CO₂ in the feed.

Maximum feed preheat temperature is 1000 °F, and there will be a feed preheat furnace expected to perform at 85% efficiency (efficiency = theoretical MBTU required / actual MBTU required). 80% of the total variable energy costs for the SU are projected to be from actual preheat furnace firing duty, with the balance to be equally divided between 125 PSIG Steam and electricity.

A basic flowsheet for the SU is:



Air Separation Plant

You are able to purchase oxygen from a third-party oxygen plant. The oxygen is supplied as 99% pure with 1 mol% nitrogen. The Air Separation Plant owner has offered the following contractual terms:

- Oxygen (500 psig, 99 % purity, 75F): \$100/short ton contained oxygen

Energy for oxygen plant pumps and compressors to be provided by customer as follows:

- Electricity Option: 1000 KW-h/short ton contained oxygen
- 600 psig Steam Option: 10,000 lb/short ton contained oxygen

The Air Separation Plant is designed so that the choice of electricity or steam shall be determined by customer. Cooling water requirement is to be provided by the customer at 400 gpm per short ton/day of oxygen.

Hydro-Isomerization Unit

The HI unit for the GTL process is to be downstream of the FTR. After initial separation of products from the FTR, the distillate and heavier boiling fractions (material with greater than 350F boiling point) are fed to a catalytic hydro-isomerization reactor, where the paraffins are isomerized and wax is converted to lighter products.

The process converts 100% of the >700F boiling point (b.p.) material to <700F b.p. material, with an overall selectivity of 1.0 wt% methane, 0.5 wt% ethane, 3.5 wt% propane, 3.5 wt% butane, 25 wt% naphtha, and the balance diesel.

Yields are expressed as overall reactor products, based on the amount of 700+ in the feed. For example:

<u>Feed</u>	<u>Basis</u>	<u>Product</u>
C1		70*1%
C2		70*0.5%
C3		70*3.5%
C4		70*3.5%
Naphtha		70*25%
Diesel	30	balance
700+	70	zero

The HI catalyst selected for this unit is very selective to >700F b.p. material. You are to assume that any <700F b.p. material in the feed to the HI will essentially pass through the HI unit and remain unconverted. The catalyst is sensitive to H₂O and CO; therefore, the liquid feed to the hydro-isomerization reactor must not have any free water above the solubility limit and the makeup gas should have a CO content no greater than 0.1 mol%.

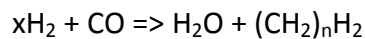
The utility and make-up hydrogen requirements for the HI Unit are:

- Fuel gas: 0.08 MBTU/bbl of feed
- Hydrogen: 300 SCF/bbl of feed
- Steam (125 PSIG): 10 lbs/bbl of feed
- Electricity: 2.5 KW-hr/bbl of feed
- Cooling Water: 300 gal/bbl of feed

FTR Unit/GTL Fischer-Tropsch Reaction

Reaction

In the FTR, the syngas is converted to hydrocarbons and water by the following reaction:



CO Conversion Kinetics

Your company has developed an ultra-stable Cobalt-based FTR catalyst that you are evaluating for a proposed commercial plant. In lab tests it was determined that the overall rate equation is best fit by a Langmuir-Hinshelwood form with parameters as follows (7):

$$-r_{CO} = \frac{k T_1 P_{H_2} P_{CO}}{(1 + k_2 T_2 P_{CO})^2}$$

$$T_1 = \text{Exp}[-4492 * (1/T - 1/473)], T \text{ in deg K}$$

$$T_2 = \text{Exp}[8237 * (1/T - 1/473)], T \text{ in deg K}$$

$$k = 0.0173 \text{ gmol CO / hr, cc cat, atm}^2$$

(catalyst bulk density = 0.8 g/cc)

$$k_2 = 4.512 \text{ atm}^{-1}$$

$$P_{H_2}, P_{CO} = \text{partial pressures in vapor phase, atm}$$

$$T = \text{Reactor operating temperature}$$

For estimation of vapor phase components in the kinetics, you may assume that the vapor phase contains 100% of the H₂, CO, H₂O, CH₄, N₂ components, and 0.7 moles of C₂+ hydrocarbon for every mol of CH₄ made.

The reaction temperature will be determined by the feed temperature, the heat of reaction and heat transfer out of the tube and may vary along the length of the reactor. Information on heat transfer characteristics is provided below.

Product Selectivity

You can assume the products of the hydrocarbon synthesis reaction are all alkanes. The distribution of C₅+ products is characterized by the Anderson-Shulz-Flory (ASF) probability distribution as follows:

$$W_n/n = [(1-\alpha)^2 / \alpha] \alpha^n$$

or,

$$M_n = (1-\alpha) \alpha^{n-1}$$

α = ASF chain growth parameter

W_n = relative weight fraction of carbon number n

M_n = relative mol fraction of carbon number n

The selectivity of methane does not follow the ASF distribution, but instead is dependent upon temperature over the range of 390-450°F as follows:

$$S_{CH_4} = r_{CH_4}/-r_{CO} = (0.03)T_3 \quad (\text{mols/mol})$$

$$T_3 = \exp[-10000(1/T - 1/473)], \quad T \text{ in deg K}$$

The ASF parameter is slightly temperature dependent and varies with the average reactor temperature as follows:

$$\alpha = (0.93)T_4$$

$$T_4 = \exp[250(1/T - 1/473)], \quad T \text{ in deg K}$$

The selectivity of C2-C4 alkanes are linked to CH4 selectivity as follows:

$$S_{C_n} = (0.04)S_{CH_4} \quad \text{mol/mol} \quad n=2,3,4$$

You have found that, typical for cobalt based catalysts, CO₂ selectivity is negligible.

Catalyst

The catalyst you will be using has been formulated into 1/16 inch diameter extrudates, with a packed bulk density of 0.8 g/cc and a void fraction of 0.4. Equivalent diameter is 0.08 inches. Cost is \$10/lb. Assume replacement every 4 years.

The catalyst is an ultra stable formulation - with low deactivation rates - and the activity (as set by the kinetic equation) can be taken as the average activity for the life of the catalyst.

Reactor Engineering

Because the reaction is highly exothermic you have selected a tubular fixed bed reactor cooled by boiling water. You have found that a practical limit for the size of these reactors is 20 ft in diameter and 60 ft in length (tangent to tangent). You need to determine the number of reactors needed and the optimum arrangement of the reactors (number of stages in series and number or reactors per stage).

Reactor Heat Transfer

The reaction is highly exothermic, with a heat of reaction of 70,200 BTU/lb mol CO converted. Temperature is controlled by adjusting boiling water pressure on the shell side of the tubular reactor. Normal operating conditions for both process and shell sides should be optimized to maximize process performance and minimize investment costs. You may assume, for this problem that the shell side operates isothermally.

You have determined that the heat transfer coefficient is controlled by process side conditions and found that an empirical relationship exists for the overall coefficient as follows:

$$U_0 = 0.385 * G^{0.8} / D^{0.2}$$

U_0 = Overall heat transfer coefficient, BTU/hr,F,ft²

G = Inlet gas mass velocity, g/hr/cm²

D = Tube diameter, cm

You may consider tube diameters in a range of ¾" to 2". Minimum spacing between tubes is 1".

Reactor Pressure Drop

Bed pressure drop should be calculated and pressure loss should be accounted for in the kinetics. Assume fluid properties are constant through the reactor and are equal to the properties at the inlet, neglecting the reaction. To account for the contribution of the liquid on overall pressure drop, assume total pressure drop is 1.5 times the gas phase pressure drop. Maximum allowable pressure drop per reactor is 50 psi.

Mass Transfer

You have found that due to the particular formulation of your catalyst that mass transfer effects are small and can be ignored.

Feed Temperature Control

The temperature of the syngas from the SU must be lowered before being fed to the FTR reactor(s). It is recommended that this is accomplished using a waste heat boiler (steam generator) in series with an air or water cooled heat exchanger.

Product Separation

You will need to design the facilities to separate the desired products in the reactor effluent from unconverted feed and water. Distillate and heavier boiling (350°F+) fractions are solid at room temperature and must be kept above 250 °F prior to isomerization to prevent wax crystallization. Naphtha and lighter components can be collected for direct shipment without temperature concern. Water should be separated for disposal and/or reuse.

Utilities

The SU, HI unit, Air Separation Plant and FTR unit will all have full access to your company's utility grid, which can provide and (in some cases) accept any utilities generated during the process, provided that specific conditions are met. If multiple hydrocarbon streams produced in the process are used as fuel gas, then each

hydrocarbon stream will be valued at its respective BTU/lb heating value. Typical cooling water make-up rate is 0.025 gallon make-up per gallon of water circulating. The boiler feed water blowdown rate is 3% of total mass of steam produced. Boiler feed water blowdown cannot be reused for boiler/steam, but can be used as cooling water make-up. Carbon dioxide may not be returned for credit.

Preliminary Design Package Requirements:

- 1) Title Page
- 2) Table of Contents
- 3) Executive Summary (w/ specific reference to design objectives)
- 4) Introduction
- 5) Summary
- 6) Discussion
- 7) Conclusions
- 8) Recommendations
- 9) Project Premises
- 10) Heat and Material Balance
- 11) FTR Unit Process Flow Diagram
- 12) Simplified GTL Plant Process Flow Diagram - Illustrating heat integration and stream flows & compositions between all units in GTL plant
- 13) Safety/Environmental Summary
- 14) Equipment Information Summary – with enough design information to cost equipment
- 15) Unit Control and Instrumentation Description
- 16) Economics - In addition to DCF, include a summary of operating costs, utility requirements and energy efficiency
- 17) Engineering Calculations, Computer Simulation Outputs
- 18) References

Additional Information:

- 1) Standard conditions are 60F and 14.7PSIA.
- 2) Your company uses US Customary Units of Measure (see utility costs).
- 3) $G = 10^9$, $M = 10^6$, $K = 10^3$
- 4) Short ton = 2000lb; bbl = barrel of liquid at standard conditions = 42 gal
- 5) Ambient: 75F (Avg), Min/Max Dry Bulb Temp = 20/90, Avg. Windspeed = 10mph.

Feed Costs:

- Methane Feed: \$2000/MSCF

Capital Recovery:

- Syngas unit: \$400M/yr
- HI unit: \$100M/yr

Utility Values:

- 600#, 490F HP Steam: Cost: \$5/klb consumed, Credit: \$4/klb produced
- 125#, 353F MP Steam: Cost: \$4/klb consumed, Credit: \$3/klb produced
- 20#, 260F LP Steam: Cost: \$3.5/klb consumed Credit: \$2.5/klb produced
- Electricity: Cost: \$0.04/KW-h consumed, Credit: \$0.03/KW-h produced
- Fuel Gas: Cost: \$3/MBTU consumed, Credit: \$2/MBTU produced
- Hydrogen: Cost: \$0.06/lb consumed
- Carbon Dioxide: 100% pure (500PSIG & 100F): Cost: \$400/MSCF consumed
- Steam Condensate (at least 99.9% v/v pure): Credit: \$2/klb produced
- Process/Cooling Tower Water (at least 95% v/v pure): Cost: \$0.5/kgal consumed, Credit: \$0.35/kgal produced
- Waste Water Treatment (at least 75% v/v pure): Cost: \$6/kgal produced

Hint: Steady-state design may not require all utilities. You may ignore transient start-up requirements for preliminary design.

Product Prices:

Product is to be transported to existing storage tanks and then loaded on to vessels for transport. The planned price structure and standard liquid densities for finished products are:

- LPG (C3, C4) – regardless of composition: \$0.30/lb

- Naphtha (C5 - C10); 45 lb/ft³: \$75/bbl
- Diesel (C11 – C20); 53 lb/ft³: \$90/bbl

Pseudocomponents:

For simulation purposes, you may consider lumping some of the product species together as pseudocomponents. The following properties are provided for suggested lumped species:

Pseudocomponent Properties					
Carbon Range	C21-C25	C26-C29	C30-C35	C36-C47	C48+
MW	322.6	386.5	454.9	572.2	861.7
SG @ 60F	0.801	0.810	0.818	0.827	0.839
NBP, F	714.3	799.6	876.7	982.5	1155.2

Additional References

- 1) Advanced Natural Gas Engineering, Wang, Xiuli; Economides, Michael © 2009 Gulf Publishing Company.
- 2) Carbon Capture and Storage, Rackley, Stephen A. © 2010 Elsevier
- 3) Future Energy – Improved, Sustainable and Clean Options for Our Planet, Letcher, Trevor M. © 2008 Elsevier.
- 4) Gasification (2nd Edition), Higman, Christopher; van der Burgt, Maarten © 2008 Elsevier.
- 5) Metal-Catalysis in Industrial Organic Processes, Chiusoli, Gian Paolo; Maitlis, Peter M. © 2006 Royal Society of Chemistry.
- 6) Wiley Critical Content – Petroleum Technology, Vol 1 – 2 © 2007 John Wiley & Sons.
- 7) Yates, I.C. and Satterfield, C.N., “Intrinsic Kinetics of the Fischer-Tropsch Synthesis on a Cobalt Catalyst”, Energy and Fuels, Vol. 5, 1991, 168-173.