



# **National Student Design Competition 2013**

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Michael D. Ackerson, Professor  
Jamie A. Hestekin, Professor

Please read the rules **before**, **during** and **after** preparing and submitting the solution to AIChE.

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# AIChE National Student Design Competition 2013

## Comparison of Bio-mass to Bio-oils Reactor Systems: Direct Conversion vs. Companion Coal Gasification

DEADLINE FOR **ELECTRONIC SUBMISSION** TO AIChE IS MIDNIGHT, June 3, 2013.

Send a WORD file and a PDF file of each entry to Michelle S. Marsnick [micma@aiche.org](mailto:micma@aiche.org)

**\* DO NOT mail any paper copies.**

### RULES OF THE CONTEST

Any significant deviation from the mandated Table of Contents and Individual Section Contents, included at the end of this Problem Statement, will result in report rejection, resulting in a Rejection Letter (citing unacceptable documentation) sent to the competitor's institution.

Solutions will be evaluated using primarily the following grading criteria.

- Suitability of process equipment.
- Correctness of results and accuracy of computations.
- Soundness of conclusions.
- Sound economic analysis, leading to an economic optimum.
- Ingenuity and logic.
- Appropriate presentation, grammatically correct but succinct and to the point.

The statement of the problem contains all the pertinent information except for that available in handbooks and other literature references. The Web (WWW) will be a valuable resource. 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. If students use commercial or library computer programs or other solution aids, they should so state in their reports and include proper references and documentation.

The 2013 National Student Design Competition is designed to be solved either by an individual chemical engineering student working entirely alone, or a team of no more than three students. Solutions will be judged in two categories: individual and team. At the sole discretion of the Judges, up to 3 winning solutions (i.e., 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> places) will be determined for individual entries and for team entries.

There are other approaches to using the problem, and it is expected that some Advisors will use the problem as classroom material and students will not follow contest rules. The following confidentiality rules therefore apply:

#### Students submitting solutions:

The problem may not be discussed with anyone (student, faculty, or others, in or out of class) before or during the period allowed for solutions. Discussion with faculty and students is permitted only after complete final reports have been submitted to the Chapter Advisor.

#### Students not submitting solutions:

Discussion with faculty and with other students who are not participating in the contest is permitted. However, if any individual or team, at the competing college or university, is solving

the problem under competition rules, rigorous and foolproof procedures must be established to prevent any communication between those competing under contest rules and those students using the problem otherwise.

All students:

The problem may not be discussed with students or faculty from other colleges or universities, or with individuals in the same institution who are still working on the problem under contest rules, until after **June 3, 2013**. This is particularly important in cases where neighboring institutions may be using different schedules.

## RULES FOR SUBMITTING SOLUTIONS

### ELIGIBILITY

- ONLY AIChE NATIONAL **ENROLLED. UNDERGRADUATE** STUDENT MEMBERS MAY SUBMIT A SOLUTION. Non-member entries will not be considered.
- Entries may 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, for electronic (WORD & PDF) submission to AIChE.

### TIMELINE FOR COMPLETING THE SOLUTION

- Students are allowed no more than thirty six (36) days (and 5 weekends) to complete the problem. 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 submitted electronically to AIChE no later than midnight, June 3, 2013.
- THE FINISHED REPORT MUST BE SUBMITTED TO THE FACULTY ADVISOR WITHIN THE 36-DAY PERIOD.

### REPORT FORMAT

- THE REPORT MUST NOT EXCEED 125, NUMBERED PAGES. ANY REPORT EXCEEDING 125 PAGES AND/OR WITHOUT ALL PAGES NUMBERED IN THE LOWER RIGHTHAND CORNER WILL BE RETURNED TO THE FACULTY ADVISOR.
- The Supporting calculations and other appendix material may be in pencil or pen; however, they must be scanned (JPEGs, 96 ppi should suffice) using the lowest resolution which is clearly legible in the report.
- The report should not contain any reference to the student's names or institution identification. Any report insert which names or otherwise identifies the institution must be avoided.

### SENDING THE SOLUTION TO AIChE

- The report(s) must be submitted as (1) a WORD file and (2) a PDF file to Michelle S. Marsnick (micma@aiche.org), by the Faculty Advisor, no later than June 3, 2013.
- Each entry must be accompanied by the enclosed ENTRY FORM giving each contestant's name, AIChE membership number, college or university, Faculty Advisor name, address, home address, home telephone number, and student chapter, electronically attached to the report. This form is used by AIChE for identification. This form must be e-mailed to Michelle S. Marsnick (micma@aiche.org) at AIChE.
- The DEADLINE: Entries must be sent in electronic form before 12:00 midnight June 3, 2012.

# 2013 AIChE National Student Design Competition: Comparison of Bio-mass to Bio-oils Reactor Systems: Direct Conversion vs. Companion Coal Gasification

## CONTEST PROBLEM STATEMENT

DATE: November 1, 2012  
TO: P. E. Fair, B. E. Peters, S. E. Walas  
FROM: P. D. Superior  
SUBJECT: Project Assignment – Evaluation of Bio-oils Reactor Systems

Good news: the bio-oils reactor(s) project has just been funded. Paul, Brian and Selena you have been selected to be the team which executes the project. We must move fast; consequently, you will be given the background information in this document to allow you to start immediately and rapidly complete the project definition.

### INTRODUCTION

“The United States consumed 18.8 million barrels per day (MMbd) of petroleum products during 2011” ([http://www.eia.gov/energy\\_in\\_brief/foreign\\_oil\\_dependence.cfm](http://www.eia.gov/energy_in_brief/foreign_oil_dependence.cfm)); however, the US produces 10.3 MMbd; thus, we import 45% of our petroleum products. All of our US presidents back to Richard Nixon and other energy experts realized that our dependence on foreign oil places our nation at risk (<http://www.youtube.com/watch?v=kbW7brZ2nds>). The DOE has funded a study which states (1 & <http://www.eesi.org/doe-releases-report-us-biomass-supply-potential-11-aug-2011>), “...found that the United States could produce more than a billion bone-dry tons of biomass from agriculture and forestry – enough to displace 30 percent of U.S. petroleum use.” Our government realizes that coal and biomass must be used to decrease our dependence on foreign oil. Higman et al. (8) have reviewed all gasification technology; Bartis et al. (3) has reviewed the technology for converting coal to liquid fuels; Tarka (15) has reviewed the technology for converting coal/bio-mass to liquid fuels and Ringer et al. (14) have reviewed the technology for converting cellulosic bio-mass to bio-oils. DOE is proposing to fund projects (<http://www.grants.gov/search/search.do?mode=VIEW&oppId=168173>) titled, “Small Scale Coal-Biomass to Liquids (CBTL) Production and Feasibility Study of a Commercial Scale CBTL Facility”, FON: DE-FOA-0000703.

The preferred technology (which is closer to commercialization or is actually commercialized) for converting coal and bio-mass to liquid fuels is pyrolysis followed by purification of intermediates with subsequent reactions to produce the desired liquid fuels.

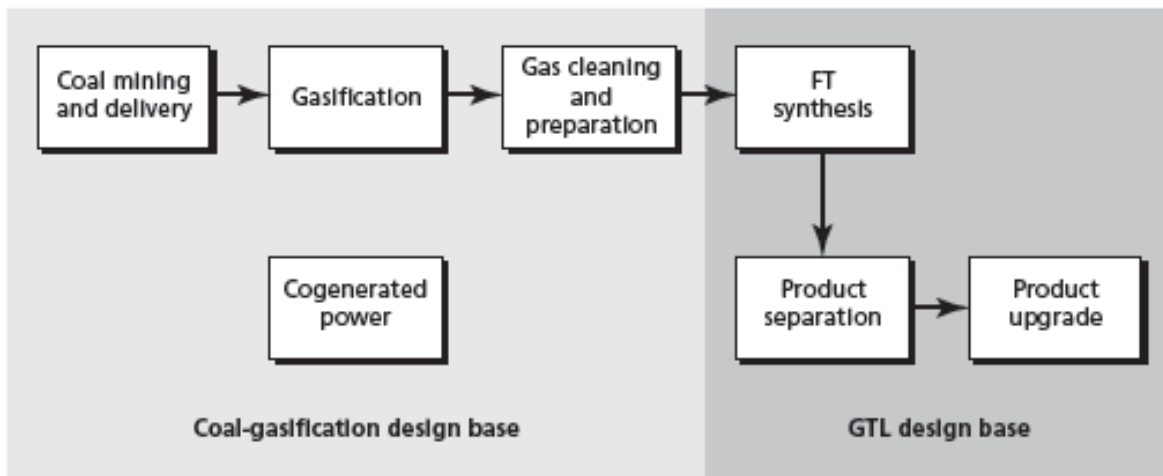
There are several Universities and National Laboratories throughout the world that research the conversion of biomass to commercial products. Information about most of them can be found on the Pyrolysis Network (<http://www.pyne.co.uk/>, see in particular “Country reports updates/Reviews of state-of-the-art”). With this background information the foundation for this 2013 AIChE Contest Problem can be firmly established.

### PROCESS TECHNOLOGY

#### Coal Pyrolysis to Liquid Fuels

A simplified schematic of the Fischer-Tropsch (FT) Coal to Liquid (CTL) process is shown in Fig. 1. Bartis (3) states, “The process begins with the gasification of coal, which consists of reacting coal with

steam and oxygen at elevated temperatures (1,000 to 1,500 degrees Celsius) and moderate pressures (~500 pounds per square inch [psi]) to produce a mixture of hydrogen, carbon monoxide, and carbon dioxide. A gas consisting mainly of the first two of these constituents is called synthesis gas. But as it leaves the gasifier, the gas is dirty: It contains carbon dioxide and various gaseous molecules that derive from the impurities found in coal. These impurities would harm the performance of subsequent processing steps and are therefore removed in sections of the FT CTL plant that are designed to clean and properly prepare the synthesis gas. Sulfur compounds are reduced to near-zero concentrations. In general, the captured sulfur would be converted to pure solid sulfur or sulfuric acid, both of which are articles of commerce as opposed to wastes. It is also during gas cleaning that extensive removal of trace mercury compounds would occur. A consequence of gas cleaning and preparation is a highly concentrated stream of carbon dioxide. In the absence of a greenhouse-gas management requirement, this carbon dioxide would be released into the atmosphere. The next step is to send the cleaned synthesis gas to FT reactors, where it is catalytically converted to a mixture of hydrocarbons. This mixture generally includes hydrocarbon gases, such as methane and propane; and hydrocarbons that are typically found in gasoline, diesel, and jet fuel; and heavier compounds that are categorized as waxes. These various streams are separated, primarily according to their boiling points, and can be further treated to produce two product streams: naphtha and middle distillates. At the FT CTL plant, the middle-distillate product can be retail-ready diesel fuel or a combination of diesel fuel and jet fuel. The naphtha product is basically a very low-octane (i.e., about 40 octane) gasoline that must be extensively upgraded before it can be used as an automotive fuel.”



NOTE: GTL = gas to liquids.

RAND MG754-3.1

Figure 1. Simplified Schematic of the Fischer-Tropsch (FT) Coal to Liquids (CTL) process (From 3, p. 16)

Zheng and Furinsky (17) have done ASPEN simulations of four coal gasifiers and they have the following to say about the operation of the Shell gasifier and the performance of the Shell and Texaco gasifiers. They have also studied the British Gas Lurgi (BGL) and the Kellogg-Rust-Westinghouse (KRW) gasifiers.

Table 1  
Typical operating parameters of gasifiers

	Shell	Texaco	BGL	KRW
Bed	Entrained	Entrained	Moving	Fluidized
Feeding	Dry	Slurry	Wet	Wet
Temperature, °C	2000	1250–1550	2000	870–1040
Pressure, Mpa	3.0	4.1	2.5	2.1
Coal size, mm	<0.1	<0.1	4–5	<5

### 2.1. Shell gasifier

Pressurized coal, oxygen and, if necessary, steam enter the gasifier through pairs of opposed burners. The gasifier consists of an outer pressure vessel and an inner water cooled membrane wall. Gasification temperature is controlled by the cooling coils where saturated steam is generated. The raw gas (mainly H<sub>2</sub> and CO) leaves the reactor at near gasification temperature. It is subsequently quenched by a cool recycle gas before entering the convective cooler where superheated steam is generated. After leaving the syngas cooler, the cooled gas passes through the bag filter where about 98% of the fly slag is removed. Part of the cleaned gas is used as quench gas. The remainder of the gas enters the scrubber to remove particulates, ammonia and salts.

The results in Tables 4 and 5 illustrate the effect of the different gasifiers on the compositions of the four gaseous streams obtained from coal A. As expected, the fuel gas from the slurry fed gasifier contains more CO<sub>2</sub> and H<sub>2</sub> and less CO than that from the dry fed gasifier because the excess of steam is consumed in the following reaction:

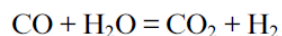


Table 4  
Conditions of various gases of Shell and Texaco processes

Component (mol%)	Shell				Texaco			
	Raw	Clean	Acid	Stack	Raw	Clean	Acid	Stack
O <sub>2</sub>	0	0	0	12.5	0	0	0	11.5
N <sub>2</sub>	4.1	4.2	0	75	1	1.3	0	75.5
H <sub>2</sub>	27.6	28.8	0.2	0	28.6	36.1	0.1	0
CO	61.3	63.8	2.3	0	38.4	48.3	0.7	0
CO <sub>2</sub>	2.2	2	21.5	6.9	12.6	12.9	69.4	7.1
H <sub>2</sub> O	2.5	2	0	4.7	17.4	0.2	0	5.1
CH <sub>4</sub>	0.1	tr	0	0	0.15	tr	0	0
Ar	0.8	0.9	0	1	0.7	0.9	0	1
H <sub>2</sub> S	1.15	6*	75.9	0	0.96	4*	29.8	0
SO <sub>2</sub>	0	0	0	<1*	0	0	0	<1*
COS (ppm)	848	44	0	0	412	25	278	0
Average molecular weight	21.1	20.9	36	29.3	30	20.8	40.9	29.2
Total volume, 10 <sup>3</sup> m <sup>3</sup> /h	31.3	6.9	2.1	2093	30.4	7.4	5.8	1989
Temperature, K	1811	311	322	378	1644	311	322	380
Pressure, bar	36	27	1.5	1	44	27	1.5	1

\* Values in ppm.

**Note:** Table 5 (not included) presents “Conditions of various gases of BGL and KRW processes”

The Texaco Gasifier produces the highest ratio of H<sub>2</sub> to CO (i.e., 0.75 vs. 0.45 for the Shell gasifier); thus, it will be used as the gasifier which supplies the hot gases required to heat the biomass to reaction temperature. In the combined process which includes the coal gasifier as the front end and the biomass

reactor as the backend, additional H<sub>2</sub> will be required to achieve the approximate 2:1 ratio of H<sub>2</sub>:CO for the Fischer-Tropsch reaction. This H<sub>2</sub> in the US would logically be supplied by reforming methane from natural gas.

## **BIO-MASS PYROLYSIS**

Ringer et al. (14) explain the fundamentals of bio-mass pyrolysis, *“Three primary products are obtained from pyrolysis of biomass. They are char, permanent gases, and vapors; that at ambient temperature condense to a dark brown viscous liquid. While pyrolysis of biomass has been practiced in some form for thousands of years, it wasn’t until recently that the relationship between heat transfer rates into the biomass and product distribution yields were well understood. The practice of charcoal manufacture from biomass is generally referred to as a slow pyrolysis process based on the rate in which heat is imparted to the biomass. The distribution of products between liquid, char, and gas on a weight basis for this “slow” pyrolysis is approximately 30%, 35%, and 35% respectively, whereas under “fast pyrolysis” conditions the product distribution is dramatically altered and shifts the distribution primarily to a liquid bio-oil product. Under these conditions bio-oil yields of liquid, char, and gas are 75%, 12%, and 13% respectively [4]. It is generally recognized that two primary processing steps are required to meet the conditions for fast pyrolysis. They are:*

- *Very high heat flux to the biomass with a corresponding high heating rate of the biomass particle.*
- *The heat transfer to the biomass must occur in a very short time period with immediate quenching following product formation.*

*The rate of the heat transfer to the particle needs to be between 600-1000 W/cm<sup>2</sup> [12]. Some unpublished work done at SERI (now NREL) in the early 1980s indicated that the heat of pyrolysis (energy required to thermally break the macro polymer bonds) was relatively low, on the order of 230 KJ/kg. The reproducibility of the data was not very good so the accuracy of this number is questionable. Other published data report numbers as high as 1000 KJ/kg.... For comparison, the amount of energy needed to reform methane to hydrogen is about 750 MJ/kg. Even at the higher value these numbers imply that once the reaction vessels are brought up to temperature the amount of energy required to actually break apart the biomass is not significant. The energy needed to carry out this transformation is readily available in the coproducts of pyrolysis gas and/or char.”*

Bridgwater and Peacocke (5) have well covered the experimental and commercial fast pyrolysis facilities and they discuss the process, the processing conditions and the products; they mention 37 facilities which have operated to study and commercialize fast pyrolysis of biomass. These processes will not be discussed in detail here as Bridgwater and Peacocke have given adequate coverage.

Figure 2 presents a process flow schematic of the Ensyn Rapid Thermal Processing unit; this illustration was taken from (5, p. 31). The Ensyn WEB site (<http://www.ensyn.com>) presents more information about the Ensyn technology and about Fast Pyrolysis of Biomass in general. The Ensyn technology was selected to highlight here because it is either near or at commercial economical operation. Bridgwater and Peacocke (4) mention 8 operational units operated by Ensyn and they describe the Ensyn process, *“The heart of the system is a transported bed reactor which contacts hot recirculated sand with biomass in an upflow reactor. In all systems, biomass is comminuted to – 6 mm and dried to not more than 10% moisture before feeding to the reactor. The products are passed through two cyclones to separate solids, then the vapour is rapidly quenched and cooled in a multiple stage system. The total residence time of the hot vapours can be controlled down to a few hundred milliseconds which ‘freezes’ the thermally unstable liquid intermediates of pyrolysis. These very low residence times are used for chemical production, while longer residence times are used for liquid fuels in order to completely crack the lignin. ....From woody biomass feeds, the overall liquid yield is up to 83% by weight on a dry basis and has typical characteristics as listed in Table 17....”* **Note:** Table 17 (5, p. 32) is presented below exactly as it appears in the original reference.



Physical property	Typical value	Range
Moisture content	22%	14–31%
pH	2.5	2.1–3.4
Specific gravity	1.18	1.16–1.22
Elemental analysis (moisture free)		
C	56.4%	55.3–63.5
H	6.2%	5.2–7.0
O (by difference)	37.1%	39.43–28.98
N	0.2%	0.07–0.39
S	< 0.01%	0.00–0.05
Ash	0.1%	0.04–0.25
C/H molar ratio	0.76	0.89–0.76
C/O molar ratio	2.02	1.87–2.92
HHV (moisture free basis)	23.1 MJ/kg	22.1–24.3
HHV as produced	17 MJ/kg	15–19
Viscosity (@40°C)	45 cp	35–55
Kinematic viscosity		
@25°C	233 cSt	
@40°C	134 cSt	
ASTM vacuum distillation		
160°C	10%	
193°C	20%	
219°C	40%	
Distillate	50°C	
Flash point	55°C	51–58
Pour point	–25°C	
Solubility		

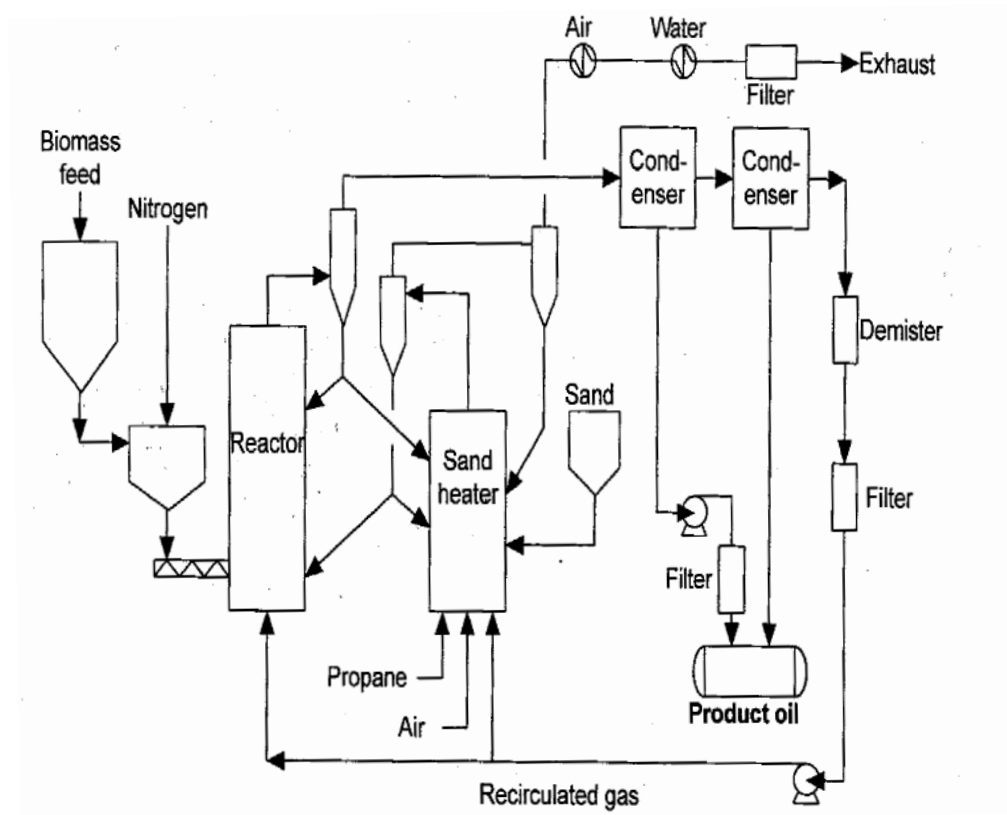


Figure 2. Ensyn RTP II Process Flow Sheet of the ENEL Bastardo Plant (Figure 11 from ref. 4)

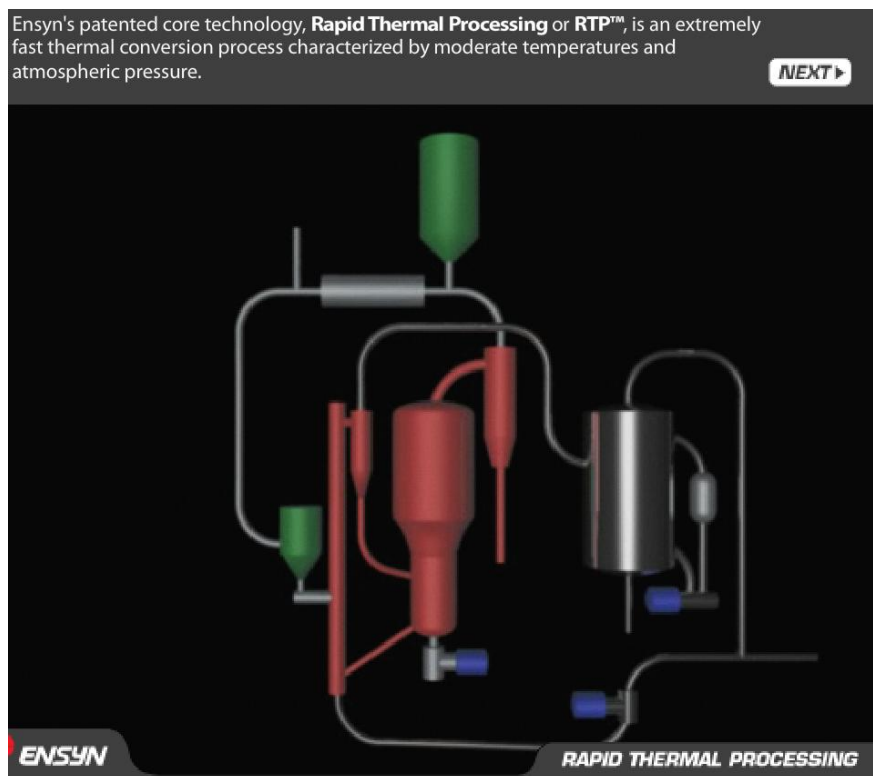


Figure 3. Schematic of the Ensyn RTP Process (From <http://www.ensyn.com/technology/overview/>)

### **STUDIES OF THE ECONOMICS OF BIOMASS TO BIO-OIL PRODUCTION**

Ringer et al. (14) have investigated the economics of producing bio-oil from 550 dry tons (2,000 lb tons)/day (1,100 delivered tons/day @ 50% moisture) of wood chips. Wright et al. (16) recently investigated the economics of producing bio-oil and biofuel in a plant converting 2,000 metric tonnes/day of corn stover to bio-oil and subsequently to bio-oil. Tarka (15) has investigated the economics of pyrolyzing mixtures of coal and biomass to produce liquid fuels. All of these studies will be very useful as a basis for doing the work required to complete the current (2013 AIChE Contest Problem) problem. All three of these studies are well documented in the references; thus, they will not be discussed further here.

### **COST SAVINGS BY 'MARRYING' BIOMASS TO BIO-OIL TO COAL GASIFICATION**

Agrawal et al. (1) have explained how one can 'marry' biomass pyrolysis with coal pyrolysis to reduce the complexity and cost of producing bio-oils while still benefiting from pyrolysis of the coal. Figure 4 from their paper shows schematically the 'married' processes. Coal is pyrolyzed (perhaps the Texaco process is economically preferred) at a pressure of 44 bar (650 psia) and 1,370 C. The hot gases from the coal pyrolysis is then rapidly mixed with a water/biomass slurry feed at the proper ratio to lower the temperature to 500 C, where the biomass will rapidly pyrolyze to bio-oil, char and gases. Rapid condensation of the offgases from the biomass pyrolysis reactor will condense the bio-oils. The produced gases will then be sent to a Fischer-Tropsch reactor or any other beneficial use device.

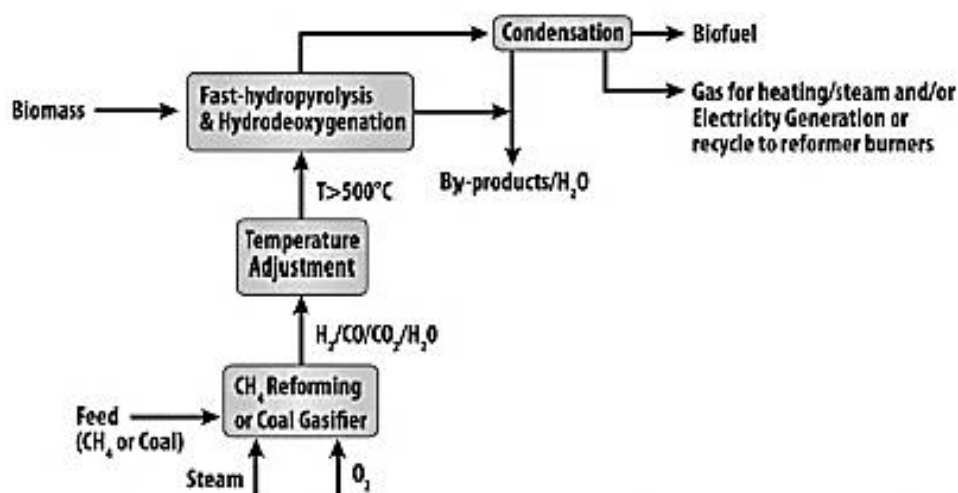


Figure 4. H<sub>2</sub>Biooil integration using direct hot syngas from a coal gasifier or a natural gas reformer.

## REQUIRED RESULTS FROM THE CURRENT WORK

The economic advantage for using the Coal/Biomass sequential reaction scheme must be determined. The most pertinent considerations for doing this study are

1. The biomass need not be dried; it can be fed as a biomass/water (perhaps 50:50) slurry.
2. The biomass need not have an intermediate heat carrier; thus, e.g., a circulating or bubbling sand bed or a hot circulating gas stream are not required.

There could be disadvantages for the ‘married’ process

1. The slag from the coal gasifier may be difficult to separate from the char from the biomass reactor.
2. More water will be in solution with the bio-oils, although there is a limit to the solubility of water in bio-oils.
3. The excess water presents a disposal or recycle problem.

Bottomline, what is needed is the cost savings (\$/lb bio-oil) for using the ‘married’ process rather than using the direct conversion process for converting biomass to bio-oils.

## ECONOMIC PREMISES

For this study a discounted cash flow analysis is probably not required. However, one needs a method for determining the capital equivalent of a yearly cash flow or the yearly equivalent of a capital investment. Use a 5 year payout for converting capital investment to equivalent yearly cash flows; i.e., a \$1,000,000 capital investment is the equivalent of \$200,000 in yearly expense.

It is, perhaps, reasonable to assume that - for a worst case scenario - the liquid products resulting from the coal gasification and conversion to biofuels will achieve a minimum IRR (perhaps 10 to 15%) required to support the capital investment in the coal conversion portion of the combined (i.e., “married”) process.

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([http://web.anl.gov/PCS/acsfuel/preprint%20archive/Files/32\\_2\\_DENVER\\_04-87\\_0068.pdf](http://web.anl.gov/PCS/acsfuel/preprint%20archive/Files/32_2_DENVER_04-87_0068.pdf))
- 14...Ringer, M. et al., "Large-Scale Pyrolysis Oil Production: A Technology Assessment and Economic Analysis", Technical Report NREL/TP-510-3779, contract number DE-AC35-99-GO10337 (2006).  
(<http://www.nrel.gov/docs/fy07osti/37779.pdf>).
- 15..Tarka, T. J., "Affordable, Low-Carbon Diesel Fuel from Domestic Coal and Biomass", DOE/NETL-2009/1349 (2009).  
(<http://www.netl.doe.gov/energy-analyses/pubs/CBTL%20Final%20Report.pdf>).
- 16..Wright, M.W., et al., "Techno-Economic Analysis of Biomass Fast Pyrolysis to Transportation Fuels", National Renewable Energy Laboratory, NREL/TP-6A20-46586, Contract No. DE-AC36-08GO28308 (November 2010).  
(<http://www.nrel.gov/docs/fy11osti/46586.pdf>).

17.. Zheng, L., Furinsky, E., “Comparison of Shell, Texaco, BGL and KRW gasifiers as part of IGCC plant computer simulations”, Energy Conversion and Management, v. 46, 1767-1779 (2005).  
<http://www.sciencedirect.com/science/article/pii/S0196890404002316>).

**FINAL REPORT FORMAT AND DOCUMENTATION**

**NOTES:**

1. FOR CONSISTENCY, CLARITY AND UNDERSTANDABILITY, ALL OF THE REPORT MUST BE DONE IN ENGLISH UNITS!
2. These formatting requirements are mandatory (non-complying reports will not be considered)
  - A. Font: 12 point, Times New Roman,
  - B. Single spaced,
  - C. Each paragraph indented,
  - D. No spaces between paragraphs
3. Every page must be numbered in the bottom right-hand corner. Section page numbers must be included in the Table of Contents.
4. **The report must not exceed 125 numbered pages.**

**Documentation Requirements**

**NOTE TO STUDENTS AND FACULTY ADVISORS:** Great difficulty was experienced while grading the 2012 NSDC Problem Team Reports. The difficulties arose because of missing, inadequate and inconsistent documentation. These documentation deficiencies increased grading (i.e., evaluation) effort and decreased grading accuracy. To improve documentation, the following documentation instructions are now MANDATORY and are not discretionary and they will be treated as such by the judges. Any significant deviation from the mandated Table of Contents and Individual Section Contents will result in report rejection, resulting in a Rejection Letter (citing unacceptable documentation) sent to the competitor’s institution.

Mandated Table of Contents: **NOTE: Every TOC Section must have its starting page # included.**

+ Title Page	
<b><u>SECTION</u></b>	<b><u>Page Number</u></b>
+ Summary -----	**
+ Introduction -----	**
+ Conclusions -----	**
+ Recommendations -----	**
+ Project Premises -----	**
+ Process Flow Diagram(s) -----	**
+ Stream Attributes Table-----	**
+ Process Description-----	**
+ Safety -----	**
+ Environmental -----	**
+ Utility Summary -----	**
+ Operating Cost Summary -----	**
+ Equipment Information Summary -----	**
+ Capital Estimate -----	**
+ Economic Analysis -----	**
+ Innovation & Optimization-----	**
+ References -----	**

+ Engineering Calculations -----	**
+ Computer Programs -----	**
+ Computer Process Simulations -----	**

The **minimum requirements** for the contents of each report section are given below.

**Title Page**

Title, Authors, Institution, Date, 2013 AIChE Contest Problem

**Table of Contents**

The report Table of Contents (TOC) must include the Report Sections exactly as listed above. The 1<sup>st</sup> page of each TOC section must be included; thus, every report page will be numbered sequentially from the 1<sup>st</sup> to the last page.

**Summary**

One page maximum condensation of the report, including project start & mechanical completion dates, project description (what was achieved & how was it achieved), environmental (how satisfied, costs), safety (how handled, costs), economics (Capital & operating costs, manpower, IRR & NPW, as appropriate), recommendations [i.e., is project implementation recommended? Is project abandonment recommended?].

**Introduction**

Orient the reader to the assigned task; it is the ideal place to include pertinent information which does not fit well into other report sections. E.g., for the 2012 Low Alcohol Beer Problem, Reverse Osmosis (RO) was the mandated technology; whereas, distillation was the original technology. The reader would be interested to know why RO replaced Distillation as the most economical technology; this section is the ideal place to inform the reader of this history. This is the ideal location for any pertinent literature surveys.

**Conclusions**

Interpret your results. Itemize your conclusions in decreasing order of significance. What do you conclude about technical feasibility? What do you conclude about economic feasibility?

**Recommendations**

Emphasize business opportunity, including potential process and other economic improvements. Mention research programs required or desired to demonstrate and/or improve the process technology.

**Project Premises**

Itemize all pertinent project, process and economic premises, including (1) start and mechanical completion dates (2) feed and product specifications, including product quality considerations (3) costs of waste treatment, raw materials, utilities, operating labor etc., (4) selling prices of all products, (5) economic parameters: including depreciation schedule, taxes, project life etc., (6) environmental requirements [e.g., De Minimis emission levels, <http://www.epa.gov/airquality/genconform/deminimis.html>] (7) processing limitations, (9) extra-ordinary costs. **NOTE: Historically, this section is the most seriously deficient.**

**Process Flow Diagram (PFD)**

It must include: (1) all process equipment items (2) descriptive names for process equipment items (3) all process streams (4) numbers assigned to all process streams (5) all utilities indicated at the location of the process equipment user and (6) the major process control loops required to control the process. Each loop includes symbols for all 3 elements of a control loop, i.e., the **Sensed Variable** [e.g., Temperature, Pressure, Composition, Flow, Level etc.], the **Manipulated Variable** [e.g., Valve Position, Pump Speed, Agitator Power, Motor Voltage etc.] and the **Controller** [e.g., Temperature, Pressure, Composition, Flow, Level, Speed etc.]. **NOTE: Historically, this section is the 2<sup>nd</sup> most deficient section.**

**Stream Attributes**

For each and every numbered process stream on the PFD, include on the PFD or in a separate table Stream Attributes (SA). SA include Stream Number, Mass Flow of Each Component, Total Mass Flow, Temperature, Pressure and Stream Volumetric Flow Rates (GPM for liquids and CFM for gases). Proper SA's (lb/hr of each component, T, P, etc.) from a Process Simulator will suffice.

### **Process Description**

For each process equipment item, explain (1) its purpose (2) how it functions to obtain the process objective [unless this is obvious, e.g., for a centrifugal pump] (3) size [e.g., 100 gpm, 50' head, 5 hp centrifugal pump] and (4) process conditions [e.g., the feed-water preheater heats 1,000 gpm of atmospheric, 100 °F boiler feed-water to 210 F using 900 gpm of 300 °F, 67 psia boiler condensate, which is cooled to 180 °F].

The strategy for controlling the process must be described. This portion of the PD can be included as each item of process equipment is described, or, perhaps preferable, it can be described in a separate subsection titled, "Process Control Strategy". **NOTE: Historically, this section is the 3<sup>rd</sup> most deficient section.**

### **Safety**

Identify and summarize the hazards associated with the **chemicals** and **process** and explain how these hazards are addressed in the design. Also comment on how this might impact capital and operating costs. **Chemical hazards** include toxicity, flammability, reactivity, bio-hazards, and others. **Process hazards** could include high pressure, temperature and others. Explain how hazards are addressed in the design. Prepare a summary table for all chemicals, including raw materials, products, intermediates, solvents, etc.; include WEB Source, NFPA numbers, Toxicity Limits, Flammability Limits, Flash Point Temperatures and waste disposal strategy [NOTE: This table is almost identical to that required for the ChemE Car Competition].

A detailed HAZOP or other hazard identification procedure is not expected - that comes later during detailed design.

NOTE: No material safety data sheet (MSDS), safety data sheet (SDS), or product safety data sheet (PSDS) is allowed within the report; This information is referenced from WEB sites; e.g., ....the MSDS for ethanol is available at (<http://www.nafaa.org/ethanol.pdf>).

### **Environmental**

Note and explain any special considerations. Explain emission limits [e.g., are De Minimis levels being used? If not, what levels are being used; how much are they above De Minimis?]. Explain and document how emission limits were achieved. Explain the economic [capital and operating costs] impact of handling environmental problems.

### **Utility Summary**

In a table, itemize each utility by user. In the table give (1) the user [e.g., Reactor Feed Preheater] (2) utility unit cost [e.g., 500 psig steam @ \$5.00/MM Btu] (3) Utility Usage Rate [e.g., 1,000,000 Btu/hr] and (4) Yearly cost [e.g., \$40,000/yr]. Sum the costs.

### **Operating Cost Summary**

In a table, itemize each cost category; give (1) category identification [e.g., Operators] (2) amount [e.g., 5/shift, 20 total] (3) unit cost [e.g., \$60,000/operator/year] (4) yearly cost [e.g., \$1,200,000 MM /yr].

### **Equipment Information Summary**

In a table, itemize pertinent information for each process equipment item. In the table give (1) the item name from the PFD [e.g., Reactor Feed Preheater] (2) Material of Construction [e.g., Carbon Steel] (3) Type & Size [e.g., 1,000 ft<sup>2</sup> (93 m<sup>2</sup>), fixed tubesheet, shell & tube exchanger] (4) process conditions [e.g., 400 F @ 300 psig] (5) Source for cost [e.g., Turton et al., Fig. A.5, p. 933] and cost [e.g., \$20,500]. Sum all the individual costs.

### **Capital Estimate**

Using the total of the purchased process equipment cost and the purchased cost of other items, use an accepted method (the Lang Factor method is adequate) for determining the total project capital requirements. Prepare a small table itemizing the results.

### **Economic Analysis**



Discuss economic methods and analysis. Include any appropriate graphical representations such as Yearly Discounted Cash Flow vs. Time. Any discounted cash flow (DCF) analysis must be presented in tabular form using the Worksheet given as Table 2, p. 306, 4<sup>th</sup> Ed., Peters and Timmerhaus. For this 2013 problem a DCF analysis is not required, because an investment equivalent strategy - using a simple 5 year payout [ $\$_{ie} = 5(\$ / yr)_{arc}$  and  $(\$ / yr)_{arc} = \$_{ie} / 5$ ] - can be used to equate capital with yearly revenues or costs.

### **Innovation and Optimization**

Explain what was done to drive the process and project towards the economic optimum.

### **References**

Example Format: 1. Turton, R. et al., "Analysis, Synthesis, and Design of Chemical Processes", 3<sup>rd</sup> Ed., Prentice-Hall, Upper Saddle River, New Jersey (2009).

### **Hand Calculations**

All pertinent hand calculations must be included. Sample calculations will not suffice. The calculations must be succinct and well documented.

### **Computer Programs**

Include Input and Output Files and an explanation of model(s) used, including nomenclature. The documentation within the programs should be adequate (for one skilled in Chemical Engineering) to understand everything within the programs.

### **Computer Process Simulations**

Include input and output files and a simulator flow chart for one set of documented process conditions for any process simulation using standard programs such as ASPEN, ChemCad or PRO/II. NOTE: THERE MUST BE A ONE-TO-ONE CORRESPONDENCE BETWEEN STREAM NUMBERS IN THE PROCESS SIMULATION AND STREAM NUMBERS ON THE PROCESS FLOW DIAGRAM. IF EXTRA STREAM NUMBERS ARE REQUIRED FOR THE COMPUTER SIMULATION, THEN USE NUMBERS FOR THESE STREAMS NOT USED ON THE PFD; I.E., STREAM NUMBERS MAY BE INCLUDED IN THE PROCESS SIMULATION WHICH DO NOT EXIST ON THE PFD.