American Institute of Chemical Engineers

AIChE®

2008 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.

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AIChE

October 2007

Dear Chemical Engineering Department Heads and Student Chapter Advisors,

I am pleased to send you the 2008 AIChE National Student Design Competition statement. Please forward it to those faculty teaching design courses. Following is this year's challenge:

"Coal to Methanol."

As always, the names of the sponsoring organization and the authors are being withheld to ensure confidentiality. Both will be announced after the deadline, June 6, 2008.

An entry form – 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.

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/.

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.

All submissions must be submitted in an electronic format – and submitted via postal mail on a cd. Submissions must be no more than two documents --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).

Solutions must be submitted **on a diskette** by postal mail or ground delivery -- postmarked no later than Friday, June 6, 2008. Please maintain a copy for your files. To order additional copies of the Student Design Competition statement, email studentchapters@aiche.org or call AIChE at 1-800-AIChemE (242-4363).

If I can be of assistance, please contact me at (212) 591-7107 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 rilong@nmsu.edu.

Thank you for your support of this important student competition.

Sincerely,

Gordon Ellis
AIChE Volunteer and Membership Activities

AIChE National Student Design Competition
2008

Rules of the Contest

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.

The 2007 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 6, 2008. 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. If you would like to become a National Student member, we must receive your membership application prior to submitting your solution. Application forms are found 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 6, 2007.
- 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 diskette to Awards Administrator, AIChE, 3 Park Avenue, 19th Floor, New York, NY 10016**

- **DEADLINE: Entries must be emailed no later than midnight June 6, 2008.**

2008 National Student Design Competition:
Coal to Methanol

Business Opportunity

The rapid rise and sustained high price of crude oil and the continuing increase in demand for chemical feedstocks fueled by double digit economic growth in the Asia-Pacific region have stimulated a world-wide industrial hunt for alternate sources of energy and chemical feedstocks.

The United States has more energy reserves in the form of coal than Saudi Arabia has in oil. Experts estimate that the US has about 265 billion tons of coal reserves. This vast amount of coal makes the US the world leader in known coal reserves.

The production of methanol from available US coal deposits has been presented as a feasible method for storing energy and a convenient intermediate for the chemicals industry. In fact, the expanded utilization of methanol has been suggested as a foundation meeting future energy needs and requirements (*Beyond Oil and Gas: The Methanol Economy*, Wiley, 2006)

You work for a company that wants to complete a technical and economic evaluation of a potential project to design, construct and operate a new world-scale methanol production facility on the Texas Gulf Coast, using coal as the primary raw material and coal gasification as the coal conversion technology. The results of your work will be considered as a primary input to the company senior leadership in deciding whether or not to proceed with developing, authorizing, and executing the proposed project.

Project Objectives

The objectives of your work are to provide a preliminary design for a coal-to-methanol process and determine the economic feasibility of the project.

Evaluation Project Scope

You are asked to complete at a minimum the following tasks and deliverables:

- Assess the project objectives, input data, boundaries, and constraints as provided to you. Document a strategy for conducting the evaluation study.
- Identify flowsheet, unit operation, and commercial technology sourcing options based on information provided to the project team, literature, and other public information sources.
- Complete a process simulation and mass & energy balance for the process in order to validate the targeted performance and as a basis for estimating capital and operating costs.
- Estimate capital and operating costs, and other significant economic factors as necessary to evaluate the overall economics of the proposed project.

- Calculate the Internal Rate of Return (IRR) for the proposed project and determine the sensitivity of the project economics with respect to changes in key input and design criteria.
- Document key considerations related to the design and operation of the proposed facility in the areas of Process Safety and Environmental performance.
- Document additional areas of recommended focus for a future project team, which were not necessary to examine in detail for the purposes of the evaluation project.

Process Description and Selected Information

Based on early investigation by your company's R&D department, it has been determined that the coal-to-methanol process you are evaluating typically includes the following process operations.

Coal Selection and Pre-Processing

Your team should select a typical source of US coal and its properties as a basis for the design. Available sources of coal, typical analysis and properties, and costs for purchase and transportation for each have been determined by your Purchasing Department, and are provided to you (Appendix 1). The spot-prices (i.e. mine mouth) for the various coal sources have already been determined by your company as follows.

Martin Lake Texas Lignite – $15.20 per ton (short ton)
Wyoming (PRB) Sub-Bituminous – $10.60 per ton (short ton)
Illinois #6 Bituminons – $32.00 per ton (short ton)

Your company has also performed a preliminary assessment of the coal transportation costs to your selected manufacturing site (Texas Gulf Coast). The estimated transportation costs are based on various modes of transportation (rail, barge, truck), which result in a variable transportation cost structure. The estimated transportation costs for the various coal sources are as follows.

Martin Lake Texas Lignite – $3.90 per ton (short ton)
Wyoming (PRB) Sub-Bituminous – $10.20 per ton (short ton)
Illinois #6 Bituminous – $6.90 per ton (short ton)

The coal feedstock requires pre-processing (e.g. crushing, sizing, drying), however, a detailed analysis of the coal-preprocessing section is not necessary. Your company has experience in coal preparation, and has estimated the costs associated with the handling and pre-processing of the coal.

Coal Pre-Processing = $ 40 / ton (short ton)

Your team can use this correlation and assume the coal pre-processing is provided as a utility and capital costs of this section need not be considered.

Coal Gasification

The gasification of coal can be represented by the following simplified reaction where the specific stoichiometry of the reaction depends on the actual coal composition.

C_xH_y + x/2 O_2 → x CO + y/2 H_2 (1)

Gasifiers operate at high temperatures (in excess of 1500 °F), and can be modeled as equilibrium reactors assuming near-complete carbon conversion using the following set of reactions.

CO + H_2O ↔ CO_2 + H_2 (2)

$$K_p = \frac{P_{CO2}P_{H2}}{P_{CO}P_{H2O}} = \frac{y_{CO2}y_{H2}}{y_{CO}y_{H2O}}$$

C + CO_2 ↔ 2 CO (3)

$$K_p = \frac{P_{CO}^2}{P_{CO2}} = \frac{y_{CO}^2}{y_{CO2}}P$$

C + H_2O ↔ CO + H_2 (4)

$$K_p = \frac{P_{CO}P_{H2}}{P_{H2O}} = \frac{y_{CO}y_{H2}}{y_{H2O}}P$$

CH_4 + H_2O ↔ CO + 3H_2 (5)

$$K_p = \frac{P_{CO}P_{H2}^3}{P_{CH4}P_{H2O}} = \frac{y_{CO}y_{H2}^3}{y_{CH4}y_{H2O}}P^2$$

These reactions and equilibrium constant expressions provide a basis to determine the relative concentrations in the gasifier product gas, assuming that the reactions are at thermodynamic equilibrium.

For flowsheeting purposes the gasifier can be approximated as an equilibrium reactor. The effluent gas composition can be determined using the above reactions, or with the equilibrium composition determined by minimizing Gibbs free energy (using a process simulator).

Your team should also select a coal gasifier design and commercial technology for your process. In selecting the gasifier technology, you will need to consider the following:

1) Select a gasifier technology which can process the selected coal type

2) Determine gasifier product rates and energy costs for modeling the entire process by considering the specified methanol production rate

3) Estimate the capital and operating costs for the selected technology

Your team will need to determine the size and number of gasifiers required for the specified methanol production rate. There are a number of open-literature sources which summarize the salient features of the various available gasifier designs. Your team may find the following reference particularly beneficial for selecting and designing a gasifier.

C. Higman and M. van der Burgt, *Gasification*, Elsevier, Amsterdam, 2003.

In addition, the authors of the preceding reference have built a companion website that includes a number of useful computer programs. The address for the companion site is as follows.

http://www.gasification.higman.de

Your team may find this website (and programs) particularly useful in performing the gasification equilibrium calculations.

Oxygen Plant

The supply of oxygen to the gasifier can be one of the most expensive parts of a gasification project. Your company has decided not to design and construct an oxygen plant to supply your process. Instead, your Purchasing Department has negotiated an oxygen supply contract with a third-party to purchase oxygen "over the fence" at the following rate:

Oxygen = $70 / Metric Ton

Acid Gas Removal

There are a number of commercial technologies available for acid gas (H_2S, CO_2) removal to treat the effluent syngas from the gasifier. Your team should select an acid gas removal technology for your process. In selecting the acid gas removal technology, you will need to consider the following.

1) Gas purity: The treated syngas should remove the sulfur to a level of 0.1 ppmv or lower

2) Selectivity: The process should have a high selectivity for H_2S relative to CO_2.

For flowsheeting purposes the acid gas removal can be approximated as a simple separation unit to the specified sulfur level of 0.1 ppmv. The separation unit should also include the amount of CO_2 that will also be removed during acid gas treating, depending on your technology selection.

Your team will need to estimate the capital and operating costs for the selected technology. There are a number of open-literature sources which summarize the salient features of the various available acid gas removal technologies. Your team may also find the following reference, as previously noted in the coal gasification section, particularly useful for identifying and specifying an acid gas removal technology.

C. Higman and M. van der Burgt, *Gasification*, Elsevier, Amsterdam, 2003.

Water-gas Shift Reactor

The syngas ratio (H_2:CO) in the gasifier product stream will likely not be at the desired stoichiometric ratio of 2:1 for the production of methanol. Your team will need to consider the design of a water-gas shift reactor to shift the syngas ratio to the desired value of 2:1. The basic chemistry in the water-gas shift reactor is represented as follows.

$CO + H_2O \leftrightarrow CO_2 + H_2$

The equilibrium constant for the water-gas shift reaction can be approximated by the following relationship.

$$\ln K_p = \ln \frac{P_{CO2} P_{H2}}{P_{CO} P_{H2O}} = \ln \frac{y_{CO2} y_{H2}}{y_{CO} y_{H2O}} = -4.33 + \frac{4577.8}{T(K)}$$

Your team will need to simulate a water-gas shift reactor in the process flowsheet, and design an appropriate reactor for your process. Your team will also need to estimate the capital and operating costs for the selected technology. The following reference may be useful in the design of your water-gas shift reactor.

J.M. Moe, “Design of water-gas shift reactors,” *Chemical Engineering Progress* **58** (1962) 33-36.

Methanol Synthesis

The methanol reactor will convert syngas into the desired methanol product. Your Research and Development department have performed a preliminary analysis of methanol synthesis from synthesis gas. The basic reaction for the synthesis of methanol is as follows.

$CO + 2H_2 \leftrightarrow CH_3OH$ (6)

The R&D team also developed an expression for the equilibrium constant for the methanol synthesis reaction (373 – 673 K).

$$\ln K_p \left(1/psia^2\right) = \ln \frac{P_{CH3OH}}{P_{CO} P_{H2}^2} = \ln \frac{y_{CH3OH}}{y_{CO} y_{H2}^2} \frac{1}{P^2} = -32.918 + \frac{11284}{T(K)}$$

The syngas, however, can also react to produce ethanol, which is a key product specification. The reaction for ethanol synthesis is as follows.

$2CO + 4H_2 \leftrightarrow C_2H_5OH + H_2O$ (8)

You can assume that ethanol is produced at a rate of 1 part per 100 parts of methanol produced.

Your R&D team has also learned that the catalysts used for methanol synthesis may also catalyze the water-gas shift reaction. In addition, they have expressed some concerns about whether the methanol synthesis actually proceeds to equilibrium. They have found the following references which provide some relevant kinetic information to help your team with the analysis and design of the methanol synthesis reactor.

G.H. Graaf, E.J. Stamhuis, and A.A.C.M. Beenackers, "Kinetics of low-pressure methanol synthesis," *Chemical Engineering Science* **43** (1988) 3185-3195. [http://dx.doi.org/10.1016/0009-2509(88)85127-3]

G.M. Graaf, J.G.M. Winkelman, E.J. Stamhuis, and A.A.C.M. Beenackers, "Kinetics of the three phase methanol synthesis," *Chemical Engineering Science* **43** (1988) 2161-2168. [http://dx.doi.org/10.1016/0009-2509 (88)87098-2]

G.H. Graaf and A.A.C.M. Beenackers, "Comparison of two-phase and three-phase methanol synthesis processes," *Chemical Engineering and Processing* **35** (1996) 413-427. [http://dx.doi.org/10.1016/S0255-2701(96)04147-5]

Your team will need to simulate a methanol synthesis reactor in the process flowsheet, and design an appropriate reactor for your process. Your team will also need to estimate the capital and operating costs for the selected technology. For the purposes of the evaluation study, methanol synthesis catalyst costs can be neglected.

Methanol Refining

The methanol your process produces must meet the AA methanol grade purity specification (Source of Reference: International Methanol Producers & Consumers Association Methanol Reference). The complete list of methanol specifications is provided in Appendix 2. For the purposes of your project, the full set of product methanol specifications can be simplified to the following:

- greater than 99.85 % w/w methanol (dry basis)
- less than 0.1 % w/w water
- less than 50 ppmw ethanol

Your Sales and Marketing department has decided that methanol will be sold into the US Gulf Coast market (assume unlimited new capacity), and determined the following methanol pricing based on these purity specifications.

Methanol pricing = $320/MT US Gulf Coast FOB

Methanol market pricing is subject to short and long-term fluctuation, therefore methanol price should be addressed in the analysis of sensitivity for the project economics.

Your team will need to simulate a methanol refining and purification process in the process flowsheet, and design an appropriate separation unit(s) for your process. Your team will also need to estimate the capital and operating costs for the selected technology

Other Information

Your R&D department has compiled a list of components and corresponding physical properties, and these are provided in Appendix 3.

The required utilities for your process, including power, steam, process and cooling water, and waste treatment, have also been estimated by your Purchasing Department. The utility costs are provided in Appendix 4.

A multitude of additional literature and public information sources are available which identify coal to methanol flowsheet and unit operation technology and sourcing options. The previous process description is intended to provide an initial framework to design a coal to methanol process, however, other variations on this process are possible. Your team is encouraged to consider other possibilities, and highlight these in the final design report.

The process design should include all required chemical and physical processing steps necessary to convert raw materials to finished products, address major by-product streams, and assure compliance with applicable environmental requirements. R&D has looked at off-site waste processing, which is included in utility cost summary. Necessary utilities and infrastructure should also be included in the process design scope.

Design Capacity

The nominal annual design should be considered as a world scale in terms of methanol production capacity.

The targeted capacity is 5000 MT per day methanol. Capital and operating costs should be included in the analysis of sensitivity for the project economics.

For the purposes of the evaluation study, each section of the plant should be sized considering appropriate over-design and/or operating configuration as necessary to address expected mechanical reliability and up-time.

Site Selection

The project team has previously examined factors such as land availability, proximity to customers, etc. and it has been decided to locate the proposed facility on the US Texas Gulf Coast. Land purchase can be neglected as a factor in the economic analysis.

By-Product Considerations

The evaluation should consider and document the necessary treatment and/or disposition of key by-products (e.g. ethanol, CO2, sulfur compounds), however by-product processing does not have to be addressed in the mass and energy balance and process design unless there is significant impact on the project economics.

Technology Selection and Conceptual Design Process

You are expected to provide a rigorous "preliminary" process design package, which will not be based on detailed equipment sizing but will be based on "rules of thumb" and other appropriate preliminary equipment sizing criteria. The intent of this evaluation project is to quantify only those issues and considerations which are necessary to obtain a meaningful technical and economic feasibility analysis of the overall project. Consideration of site integration issues, including an overall mass and energy balance, will be an important input to the economic evaluation.

You should develop a documented basis for the technologies and sourcing that are ultimately recommended for inclusion in the overall technology package.

Physical Properties and Process Simulation

You should complete a mass and energy balance of the entire process from feedstock to product. Key chemistries, products, and byproducts should be included. Appendix 3 provides the list of components that must be considered and necessary properties and calculation routes that should be employed.

Infrastructure, Utilities, and Environmental Impact

The basis of the design assumes a brown field site, i.e., the land has been primed for industrial use. Resources like raw water supply will be available from neighborhood natural resources. Electricity is available from the power grid. Air and water emissions and other environmental impact should comply with applicable regulations and standards. It is assumed that the utility and operating costs provided for waste treatment will result in waste streams which are in compliance with applicable regulations.

Other Considerations

The process design package should include recommendations and key design/operating considerations with regard to Environmental and Process Safety performance of the facility.

Judging Criteria

The results of your work will be evaluated based on the following criteria:

- Determination of the project Internal Rate of Return (IRR), based on the nominal design criteria and considering capital project execution and a 20-year period of facility operations following the Return To Operations (RTO) date.
- Consideration of the sensitivity of the project economics (IRR) with respect to changes in key input and design criteria.

- Appropriate consideration of critical factors and robustness of the proposed process flowsheet, process design, and economic evaluation.
- Effectiveness of the strategy employed for technology assessment and selection.
- Completeness of the final report, in terms of effective guidance to a future project team.

Deliverables

Final report shall include:

- Executive Summary
- Overall Project Scope Description
- Design Basis, Principles and Limitations
- Technology Selection Criteria and Conclusions
- Process Performance Summary
- Project Economics Summary
- Process Description
- Process Flow Diagram with all process equipment and all stream numbers shown
- Major Equipment List with preliminary sizing for cost estimation
- Environmental and Process Safety Considerations and Analysis
- Appendices – technology references

Appendices

1. Coal sources and composition
2. Methanol specifications
3. Component list and property data/parameters
4. Utility costs – Oxygen, electricity, steam cost and credits, and basis for economic model
5. Economic Information
6. Literature references

Appendix 1 - Coal sources and composition

Composition is expressed in weight percent.

MARTIN LAKE TEXAS LIGNITE

Proximate Analysis	As Received	Dry Basis	MAF
% Moisture	34.83	--	--
% Ash	6.92	10.62	--
% Volatiles	30.18	46.31	51.81
% Fixed Carbon	28.07	43.07	48.19
	100.00	100.00	100.00
% Sulfur, S	1.30	1.99	2.23
HHV Btu lb-1	6950		

Ultimate Analysis	As Received	Dry Basis	MAF
% Moisture	34.83	--	--
% Carbon, C	42.13	64.64	72.32
% Hydrogen, H	3.15	4.84	5.42
% Nitrogen, N	0.80	1.23	1.38
% Sulfur, S	1.30	1.99	2.23
% Ash	6.92	10.62	--
% Oxygen, O	10.87	16.68	18.66
	100.00	100.00	100.00

MONTANA SUB-BITUMINOUS

Proximate Analysis	As Received	Dry Basis	MAF
% Moisture	10.50	--	--
% Ash	11.20	12.51	--
% Volatiles	34.70	38.77	44.32
% Fixed Carbon	43.60	48.72	55.68
	100.00	100.00	100.00
% Sulfur, S	1.10	1.22	1.40
HHV Btu lb-1	8600		

Ultimate Analysis	As Received	Dry Basis	MAF
% Moisture	10.50	--	--
% Carbon, C	59.82	66.84	76.40
% Hydrogen, H	4.38	4.89	5.59
% Nitrogen, N	1.33	1.49	1.70
% Sulfur, S	1.10	1.22	1.40
% Ash	11.20	12.51	--
% Oxygen, O	11.67	13.04	14.90
	100.00	100.00	100.00

ILLINOIS BITUMINOUS

Proximate Analysis	As Received	Dry Basis	MAF
% Moisture	13.00	--	--
% Ash	10.70	12.30	--
% Volatiles	37.00	42.53	48.49
% Fixed Carbon	39.30	45.17	51.51
	100.00	100.00	100.00
% Sulfur, S	3.74	4.30	4.90
HHV Btu lb-1	11000		

Ultimate Analysis	As Received	Dry Basis	MAF
% Moisture	13.00	--	--
% Carbon, C	59.82	68.76	78.40
% Hydrogen, H	4.12	4.74	5.40
% Nitrogen, N	1.07	1.23	1.40
% Sulfur, S	3.74	4.30	4.90
% Ash	10.70	12.30	--
% Oxygen, O	7.55	8.68	9.90
	100.00	100.00	100.00

Appendix 2 - Methanol Specifications

The methanol must meet the AA methanol grade purity specification. Source of Reference: International Methanol Producers & Consumers Association Methanol Reference.

For the purposes of the evaluation study, the full set of product methanol specifications can be simplified to the following:
AA Grade Methanol
- greater than 99.85 weight % methanol (dry basis)
- less than 0.1 weight % water
- less than 50 ppm ethanol by weight

U.S Federal grade: "AA". It is expected that this methanol will meet the International Methanol Producers and Consumers Association (AMPCA) 1999 methanol reference specification. If not, please provide exceptions, and an explanation.

International Methanol Producers & Consumers Association Methanol Reference

Items	Limit	Method
Appearance	clear and free of suspended matter	IMPCA 003-98
Purity wt% on dry basis	min 99.85	IMPCA 001-98
Color Pt/Co scale	max 5	ASTM D 1209-93
Water % w/w	max 0.1	ASTM E 1064-92
Distillation range at 760 mm Hg	max 1.0°C to include 64.6° $\pm$ 0.1°	ASTM D 1078-97
Specific gravity 20°C/20°C	0.791 - 0.793	ASTM D 891-95
Potassium permangate time test at 15°C	min 60'	ASTM 1363-94
Carbonizable substances Pt/Co scale (sulfuric acid wash test)	max 30	ASTM E 346-94
Ethanol mg/kg	max 50	IMPCA 001-98
Chloride as Cl^{-1} mg/kg	max 0.5	IMPCA 002-98
Sulfur mg/kg	max 0.5	ASTM D 3961-89
Hydrocarbons	pass test	ASTM D 1722-90
Carbonilic Compound as acetone mg/kg	max 30	ASTM E 346-94
Acidity as acetic acid mg/kg	max 30	ASTM D 1613-96
Total iron mg/kg	max 0.1	ASTM E 394-94
Nonvolatile matter mg/100ml	max 10	ASTM D 1353-96

Appendix 3 - Component list and property data/parameters

During design of the operations it will be necessary to model the thermodynamics of the systems encountered.

Component List

Although different components will exist in certain areas of the process, the following list should be considered an exhaustive component list (i.e., other by-products and impurities can be neglected in the design)

Component	Formula
Water	H_2O
Nitrogen	N_2
Oxygen	O_2
Hydrogen	H_2
Carbon monoxide	CO
Carbon dioxide	CO_2
Argon	Ar
Hydrogen sulfide	H_2S
Methane	CH_4
Ammonia	NH_3
Carbon	C
Methanol	CH_3OH
Ethanol	C_2H_5OH
Coal	
Ash	

Mixture modeling

It can be assumed that the solubility of the fixed gases in the liquids follow Henry's Law. The following form should be employed:

$$\ln H = a + \frac{b}{T} + c \ln T$$

where T is in Kelvin and H is in Pa/mol fraction.

Table 1. Henry's Constants for Gases in Water

	Henry's Constants		
Component	**A**	**B**	**C**
H_2	121.99	-4882.18	-14.56
Ar	145.71	-6624.60	-17.79
N_2	157.84	-6988.17	-19.58
O_2	154.40	-7049.45	-19.05
CO	162.07	-7270.48	-20.22
H_2S	105.77	-5600.74	-12.14
CH_4	160.78	-7386.74	-19.99
CO_2	161.25	-8341.45	-20.07
NH_3	93.98	-7403.58	-10.10

Table 2. Henry's Constants for Gases in Methanol

	Henry's Constants		
Component	**A**	**B**	**C**
H_2	69.82	-1850.96	-7.61
Ar	82.65	-3024.74	-9.33
N_2	80.36	-2566.04	-9.12
O_2	83.96	-3103.43	-9.51
CO	81.75	-2885.23	-9.25
CH_4	78.04	-3030.58	-8.65
CO_2	80.32	-4196.95	-8.72

For liquid mixtures, the NRTL model can be assumed to properly capture the non-ideality in the form of an activity coefficient:

$$\ln \gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right)$$

where

$$G_{ij} = \exp\left(-\alpha_{ij}\tau_{ij}\right)$$

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T} + e_{ij}\ln T + f_{ij}T$$

$$\alpha_{ij} = c_{ij} + d_{ij}\left(T - 273.15K\right)$$

For this project, the following assumptions can be made:

$$\tau_{ii} = 0$$

$$G_{ii} = 1$$

$$c_{ij} = 0.3$$

$$a_{ij} = d_{ij} = e_{ij} = f_{ij} = 0$$

b_{ij} is unsymmetrical (i.e. b_{ij} does not necessarily equal b_{ji})

Values of b_{ij} are provided in table 3 for necessary binary pairs.

Table 3. NRTL binary interaction parameters.

b_{ij}	Methanol	Ethanol	Water
Methanol	-	-51.54	-98.78
Ethanol	36.53	-	-44.41
Water	383.48	788.45	-

Appendix 4 - Utility costs – Oxygen, electricity, steam cost and credits, and basis for economic model

MT = metric ton
Mgals = 1000 US gallons
MCF = 1000 Cubic Feet

Utilities		
HHP Steam	26.00	$/MT
HP Steam	22.00	$/MT
MP Steam	19.00	$/MT
LP Steam	15.00	$/MT
Electricity	0.07	$/KWH
Condensate	0.75	$/MT
Cooling Water Makeup	1.10	$/Mgals
Process Water	1.00	$/Mgals
Demin Water	3.00	$/Mgals
Potable Water	2.50	$/Mgals
Waste Water Treatment	1.00	$/Mgals
TOC in Waste Water	0.70	$/lb TOC
Instrument Air	0.45	$/MCF
Bulk Liquids Waste Processing	410	$/MT
Bulk Solids Waste Processing	325	$/MT
Vents/Vapors Processing	330	$/MT
Inert Gas	0.35	$/MCF

Appendix 5 – Economic information

Typical engineering references and estimation procedures should be used for estimating capital costs of equipment and evaluating the project economics.

For project economics, use the following assumptions:

- 40% Tax Rate
- 3% Inflation
- 15 year straight line depreciation
- 20 year project life
- 3% Maintenance Capital per year

For determination of the project Internal Rate of Return, consider the accumulated project capital cost as a single year 0 quantity. This can be accomplished by estimating capital costs in current year currency and eliminating escalation, capitalized interest, and cost of monies.

Appendix 6 – Literature References

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