National Student Design Competition 1995

Announcing TEAM Eligibility

*For the first time ever, AIChE will accept
entries from teams as well as individuals
See contest rules inside for details*

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
345 East 47th Street, New York, New York 10017-2395

If there are any questions about the design problem, Student Chapter Advisors and design course instructors are asked to contact:

Dr. W Roy Penney
Acting Chair, National Student Design
Competition Subcommittee
Chemical Engineering Department
University of Arkansas
Fayettevlle, AR 72701

Telephone number: 501-575-5681
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Please read the rules on the following pages carefully before submitting a solution to AIChE.

AIChE NATIONAL STUDENT DESIGN COMPETITION 1995

Production of Methanol by a New Process Utilizing Methyl Formate as an Intermediate

DEADLINE FOR MAILING

Solutions must be postmarked no later than **Midnight, June 9, 1995**.

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. **The references cited at the end of the problem statement are critical to solving the problem. Therefore, one copy of the entire set will be mailed with each order of 1995 National Student Design handbooks. Advisors are encouraged to put this information on reserve for participating students, or make additional copies as necessary.**

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 other 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. Students are further advised that the problem can be solved without the use of sophisticated computer programs. Judging is based on the overall suitability of the solutions, not on skills in manipulating computer programs.

The 1995 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 or universities, or with individuals in the same institution who are still working on the problem for the contest, until after June 9, 1995. 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.
- 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 and send these by registered mail, as per the below instructions, to the Institute.

TIMELINE FOR COMPLETING THE SOLUTION

- A period of not more than thirty 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 9, 1995.
- 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, typewritten or computer-generated. Tables may be written in ink. Supporting calculations and other appendix material may be in pencil.
- The solution itself must bear no reference to the students' names or institution by which it might be identified. In this connection, graph paper bearing the name of the institution should be avoided.

SENDING THE SOLUTION TO AIChE

- Two copies of each of the solution(s) must be sent to the below address; original manuscript(s) must remain in the possession of the Student Chapter Advisor, or Faculty Advisor, sponsoring the student(s).
- There should not be any variation in form of content between the solution submitted to the Faculty Advisor and that sent to the AIChE office.
- Each copy 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, lightly attached to the report. This form will be retained for identification by the executive director of the Institute.
- DEADLINE: Entries must be postmarked no later than midnight, June 9, 1995.
- As soon as the winners have been notified, original manuscripts must be forwarded to the office of the executive director as soon as possible.

SEND TO:
Coordinator, Student Chapter Activities
American Institute of Chemical Engineers
345 East 47th Street
New York, New York 10017-2395

DEADLINE: JUNE 9, 1995

PROBLEM STATEMENT OUTLINE

PRODUCTION OF METHANOL BY A NEW PROCESS
UTILIZING METHYL FORMATE AS AN INTERMEDIATE

INTRODUCTION

Almost all methanol is currently produced from carbon monoxide and hydrogen in fixed bed, catalytic gas-phase reactors operating at 50-100 atm and 230-270 C.

An alternate two-step, liquid-phase process has been developed which reacts carbon monoxide and methanol in a first stage reactor to produce methyl formate and then, in a second stage reactor, the methyl formate is hydrogenated to produce methanol. The reaction chemistry is:

$$CO + MeOH \ ---> \ MeF \tag{1}$$

$$MeF + 2H_2 \ ---> \ 2MeOH \tag{2}$$

Your company has been retained by a large North American energy company to investigate the technical and economic feasibility of this new process for the production of methanol using natural gas and air as the raw materials. The client has large natural gas reserves throughout North America - in the U.S., Canada, Mexico and Central America. Many of these reserves are in remote areas where pipeline transportation of natural gas to potential customers is costly. Conversion of the natural gas to liquid methanol makes transportation of a product to market more economical.

In order for the commercialization of this new technology to be pursued it must show the potential for producing methanol at prices competitive with historical pricing. A recent issue of Chemical Marketing Reporter (June 20, 1994, page 3) addresses methanol pricing. The 6/20/94 CMR list price for methanol was $.72/gallon. In the 1980's and early 90's methanol sold at a low of about $.30/gallon and an average price of about $.50/gallon. Recently, prices have stabilized at about $.75/gallon with some spot prices of $.90/gallon. If the new technology shows potential for a reasonable return on capital at the current prices, then it may be desirable to take the next logical step and do a detailed comparison with competitive process technologies.

STATEMENT OF THE PROBLEM

The study premises and the study deliverables are:

PREMISES:

1. Plant capacity: 2,400 metric tons per day.
2. Cost of methane: $0.50, $1.00 and $2.00 per MM Btu.
3. Methanol transportation cost: $0.05 per gallon.

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4. Natural gas (assume 100% methane) is available at 500 psig and 25 C.
5. The plant is "grass roots" in a remote location, thus minimal utilities are available. All prime movers above 500 HP will be driven by steam turbines.
6. Steam will be generated at 1250 psig by a natural gas fired power boiler.
7. The product methanol is 99.9% pure.

DELIVERABLES:

1. An economical plant design based on the available literature data for the two-step process.
2. A project definition report which documents the project definition work.
3. Recommendations included in the project definition report which address: a) future research program and b) additional process definition work needed to further optimize the process and project.
4. The required selling price of methanol will be determined to return an IRR of 15% as a function of natural gas price.

FINAL REPORT FORMAT

NOTE: FOR CONSISTENCY AND EASE OF GRADING, ALL OF THE REPORT MUST BE DONE IN <u>ENGLISH UNITS</u>!!!!!!!!!!!!

1. Title Page.
2. Table of Contents.
3. Executive Summary - Two (2) page condensation of report.
4. Introduction - Orient the client to the assigned task.
5. Summary - Summarize the results of the analysis and summarize the conclusions and recommendations. Briefly tell what options were considered and the advantages/disadvantages of each.
6. Conclusions - Interpret your results. List your conclusions in decreasing order of significance.
7. Recommendations - Emphasize cost reduction and future research.
8. Project Premises - Itemize all pertinent process and economic premises.
9. Process Flow Diagram (PFD) - Include all items of process equipment, include and number all process streams, indicate all utilities needed per individual equipment.
10. Stream Attributes - For each and every stream on the PFD include on the PFD or on a separate page a Tabulation of Stream Attributes, including Stream Number, Mass Flow of Each Component, Total Mass Flow, Temperature, Pressure and Volumetric Flow Rate (GPM for liquids & CFM for gases).

11. Process Description - Include process conditions, equipment type and size and how the process equipment is integrated to achieve process objectives.
12. Safety and Environmental - Note and explain any special considerations.
13. Utility Summary - Itemize each utility by user. Give yearly cost for each user and total yearly costs.
14. Operating Cost Summary - Itemize using the categories given in Peters and Timmerhaus, Fourth Edition, Tables 26 & 27, pages 210 & 211.
15. Equipment Information Summary - Itemize operating conditions and sizes of process equipment for each and every item of process equipment.
16. Capital Estimate - Itemize process equipment costs and itemize the overall estimate per Method C [1], page 180.
17. Engineering Calculations - Include all pertinent hand calculations.
18. Computer Programs - Include input and output files, an explanation of the model(s) used and nomenclature.
19. Computer Process Simulation - Include input and output files and a flow chart for one set of documented process conditions for any process simulation using standard programs such as ASPEN and HYSIM. NOTE: THERE MUST BE A ONE-TO-ONE CORRESPONDENCE BETWEEN STREAM NUMBERS IN THE PROCESS SIMULATION AND STREAM NUMBERS ON THE PROCESS FLOW DIAGRAM.

BASIS FOR PROCESS DESIGN

The client has done considerable preliminary analysis of processing alternates and, based on conclusions from these analyses, the following process design premises are established. These premises are not to be changed unless it can shown that alternate technology is more economical.

Synthesis Gas Production

The synthesis gas will be produced by low-temperature selective oxidation of methane to carbon monoxide and hydrogen (and by-product water and carbon dioxide) using catalysts and process conditions of [2]. The experimental results of this investigation, using Co/Mg fixed bed catalysts, are summarized in Table 1 of the reference. Our client has indicated that their preliminary investigation concluded that multiple reactors are desirable with intermediate cooling of the process stream with waste heat boilers producing steam.

Air Separation

The process requires rather pure oxygen, thus an air separation unit is required to provide oxygen for the partial oxidation reactor. You may assume that the air separation unit

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(ASU) operates like the unit defined in Figure 5, page 20 of [3] - the 1993 AIChE Contest Problem. That unit handled 41,000 Lbmole/Hr of air and, as indicated on page 14 [3], the 1991 capital cost of the bare ASU was $21,000,000. On page 12 of [3] the recycle nitrogen stream is given as 1/3 of the oxygen mass flow rate. As indicated in [3], the inlet air compressor and the recycle nitrogen compressor must be sized and costed.

Water and Acid Gas Removal

The carbonylation catalyst is adversely affected by water and carbon dioxide. The Rectisol process will be used to remove carbon dioxide to below 10 ppmv and water to below 1 ppmv. The principle of operation and base capital and operating costs for the Rectisol process are given on pages 4 & 6 of [4] - the Problem Statement of the 1989 AIChE Contest Problem. The capabilities of the Rectisol process are also discussed on page 24 of [10].

Separation of Carbon Monoxide and Hydrogen

This separation will be accomplished using UOP's POLYBED PSA System. This patented and trademarked system is explained in [5]. According to the authors, "Typical hydrogen product purities range from 99 to 99.999 vol %. Removal of carbon monoxide and carbon dioxide to 0.1-10 ppmv is common and easily achievable." Feed pressure requirement is 200-400 psig.

The approximate capital and operating costs for this system have been obtained from a UOP representative: "In typical hydrogen/carbon monoxide separation that produces 35 MMSCFD (NOTE: million std. cu. ft. per day) product hydrogen the capital cost would be approximately $4,000,000. Installation would add an additional 20%. This capital cost does not include any compression of the CO-rich tail gas. Our experience has shown that a scaling factor of 0.65 is more accurate than the standard 0.6. Operating costs are very low. Instrument air and some power for the control system are the only requirements. The absorbent lasts for the life of the equipment, and one man would be adequate supervision."

Carbonylation of Methanol to Methyl Formate

The research work documented in [7] will be used to design the carbonylation reactor. Methanol is recycled to this reactor(s) from the hydrogenation reactor(s). The soluble catalyst is potassium methoxide. The reaction of methanol plus carbon monoxide to form methyl formate is an equilibrium reaction; thus, there will be an optimum number of carbonylation reactors and an optimum conversion of methanol. It appears that equations 8 and 9 (for process conditions relatively far away from equilibrium) are the appropriate kinetic expression to use to size the carbonylation reactor(s).

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The level of agitation in the experimental reactor was very high, thus mass transfer of CO was not at all limiting. It will probably not be practical to operate at such a high level of agitation in the commercial reactor(s); thus, mass transfer of carbon monoxide will be important. Tatterson [6] has summarized experimental and correlational work on liquid phase mass transfer coefficients in agitated vessels. For a six-bladed disk turbine (Power Number = 5) equation 6.135 from [6] is recommended to predict the mass transfer coefficient:

$$Kla = 0.046 \times (Pg/V)^{0.54} \times (Vsg)^{0.68} \qquad (3)$$

where: Kla = Liquid phase mass transfer coefficient, 1/s
      Pg = Gassed agitator power, KW
      V = Vessel volume, cu. m.
      Vsg = Superficial gas velocity based on entering gas, m/s

Correlations for a) gassed power as a function of gas rate and ungassed agitator power and for b) flooding of a six-bladed disk impeller can be found in [6] but for the purposes of this study it will be adequate to use 0.005 > Vsg > 0.02 and assume that gassed power is 75% of the ungassed power.

The solubility of CO in methanol was determined [7] and the equation relating the partial pressure of CO to the liquid phase mole fraction of CO and temperature is given on page 189 of the reference [7].

Hydrogenation of Methyl Formate to Methanol

A kinetic expression [7] was determined for a copper-chromite solid catalyst. The rate is a function of temperature, methyl formate concentration, hydrogen and carbon monoxide partial pressures and the catalyst loading. The rates for this study were rather low, which will result in large hydrogenation reactors. A different method of catalyst reduction evidentally gives an order-of-magnitude increase in hydrogenation rate. To quote from [7], "A comparison of calculated reaction rates is shown in Fig. 6. The rate observed in this study is comparable to that reported by Monti et al. but much lower than that reported by Sorum and Onasger. Gas phase catalyst reduction was employed in this study and that by Monti it al. while liquid phase reduction was used by Sorum and Onsager. Monti et al. attributed the difference to the method of catalyst reduction."

Catalyst reduction in the liquid phase gives a much more active catalyst. Figure 6 of [7] indicates a 10 fold increase for liquid phase reduction versus gas phase reduction over the temperature range of 100-160 C for catalyst loading of 1 gm/l, a pressure of 71 bar and methyl formate concentration of 16 mol/l. For this preliminary investigation, assume that liquid phase catalyst reduction will be used to produce the most active catalyst; thus, use equation 12 of [7] as the kinetic expression for gas phase catalyst reduction but, based on the work of Sorum

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and Onsager _for liquid phase catalyst reduction, multiply this_
expression by a factor of 10. Obviously, additional research
will be required to verify that these assumptions are valid.

Catalyst Separation and Recycle

Both catalysts - the soluble carbonylation catalyst and the
heterogeneous hydrogenation catalyst - need to be recycled.
Methods must be devised to recycle each of them. The
hydrogenation catalyst is United Catalyst G-89, diameter < 6
microns. The most appropriate centrifuge is probably a disk-
nozzle type. Dorr-Oliver and Centrico are two manufacturers of
this type of centrifuge. A Dorr-Oliver representative has
supplied the following information about their disk-nozzle
machines. The maximum capacity of their largest machines is
about 650 gpm with a 250 HP drive motor. The 1995 cost of this
totally-enlcosed machine in 316 SS is about $475,000. Vita about
the next smaller Dorr-Oliver machine is: 350 gpm, 150 HP &
$325,000. Timmerhaus [1] gives cost data for centrifuges in
Figures 14-72 thru 14-74, but the cost is not given for disk-
nozzle machines. The cost of Bird Solid Bowl, Stainless
centrifuges - Figure 14-74 - is probably closest to the cost of a
disk-nozzle centrifuges for the same HP driver.

CAPITAL ESTIMATE

Working Capital - Per Table 26, page 210 of [1]

Total Installed Capital

Use Method C, page 180 [1], Percentage of Delivered-
Equipment cost.

Purchased (& Delivered) Equipment Cost

1. Heat Exchangers - Use Fixed-tube-sheet, Fig. 15-15, [1].
2. Distillation Columns - Figure 16-28, [1].
3. Process Vessels - Figures 14-58, [1] for large volume
    storage tanks and Tables 4 and 6, pages 538 and 542 for
    high pressure reactors, [1].
4. Six-Bladed Disk Turbine Agitators - Fig. 14-57, [1].
5. Power Boilers - [1] provides no data thus use page 262
    of Garrett [8]. The 1987 cost of a field erected 1250
    psig unit, from an adjusted curve fit of the Garrett
    curve for a Field Erected, 400 psig unit is: $p =
    $10,000,000 x (1E6/SR)^0.82 x 1.38, where $p is the 1987
    purchase cost of a 1250 psig field erected unit and SR
    is the steam rate in million lb/hr. To determine
    the installed cost Garrett recommends an installation
    factor of 1.21.
6. Compressors - Table 9, page 14, [3] and Fig. 14-48, [1].

7. Pumps - Fig. 14-40, [1] for single stage centrifugals.
   For multi-stage centrifugals assume the purchase price
   varies as 0.6 power of number of stages.
8. Centrifuges - See "Catalyst Separation and Recycle"
   above.
9. Air Separation - See "Air Separation" above.
10. Water and Acid Gas Removal - See "Water and Acid Gas
    Removal" above and [4], pages 4 & 6.
11. Hydrogen Separation - See "Separation of Carbon Monoxide
    and Hydrogen" above.
12. Freight - Use 5% of purchase price.

OPERATING COSTS

Refer to Table 27, page 210 [1]. Use Table 23, page 200 [1]
for Selected Utilities and Labor.

1. Raw Materials - Natural Gas: $.50, $1.00 & $2.00/MMBtu.
2. Operating Labor (OL) - Estimate the number of operator
   positions. There are 4 operators per shift position.
   Labor cost, page 200, [1].
3. Direct Supervision and Clerical Labor - 17.5% of OL.
4. Utilities - Individual determination. For steam rates
   for steam turbines see pages 5-25 thru 5-31 [9].
5. Maintenance & Repairs - 3% of Fixed Capital Investment.
6. Operating Supplies - 15% of Maintenance & Repairs.
7. Laboratory Charges - 15% of OL.
8. Patents and Royalties - $0.0005/gallon methanol
9. Local Taxes and Insurance - 3% of Fixed Capital
   Investment.
10. Plant Overhead - 60% OL, Supervision and Maintenance.
11. Administrative Expenses - 15% OL, Supervision and
    Maintenance.
12. Distribution & Selling - $250,00/year + $0.05/gallon.

ECONOMIC PREMISES

1. Cash Flow Analysis done per Table 2, page 306 & 307 [1].
   Use 1/1/99 costs to do the cash flow analysis; i.e., do
   not inflate costs year-by-year.
2. 10 year project life.
3. Required IRR = 15%.
4. Startup at full capacity 1/1/99.
5. Inflation prior to 1/1/99 = 2.5%/year.
6. Depreciation: 7 year MACRS. See page 287, [1].
7. Incremental Income Tax Rate: 34% Federal + 6% State.

REFERENCES

NOTE: IT IS ASSUMED THAT EVERY STUDENT HAS READY ACCESS TO
       THE TEXTBOOK BY PETERS & TIMMERHAUS [1]. MOST STUDENTS

WILL NOT HAVE READY ACCESS TO THE OTHER REFERENCES.
A SINGLE COPY OF REFERENCES 2-10 (OR THE PERTINENT
INFORMATION FROM [8] & [9]) CAN BE OBTAINED BY CONTACTING
AIChExpress CUSTOMER SERVICE, 1-800-242-4363.

1. Peters, M.S. & K.D. Timmerhaus, PLANT DESIGN & ECONOMICS
    FOR CHEMICAL ENGINEERS, 4'th Edition, McGraw-Hill, 1990.
2. Choudhary, V.R. et al, "Low-temperature Selective Oxidation
    of Methane to Carbon Monoxide and Hydrogen over CO-MgO
    Catalysts," APPLIED CATALYSIS A: GENERAL, 90 (1992) L1-L5.
3. "Integrated Coal Gasification Combined Cycle Power Generation
    Plant Design," 1993 AIChE National Student Contest Problem -
    Statement of Problem.
4. "Methanol Production from Partial Oxidation of Vacuum Resid,"
    1989 AIChE National Student Contest Problem - Statement of
    the Problem.
5. Miller, G.Q. & J. Stoecker, "Selection of a Hydrogen
    Separation Process," Paper presented at the 1989 NPRA Annual
    Meeting March, 1989, San Francisco, California.
6. Tatterson, G.B., FLUID MIXING AND GAS DISPERSION IN AGITATED
    TANKS, McGraw-Hill, 1991.
7. Liu, Z. et al, "Kinetics of Two-Step Synthesis in the Slurry
    Phase," Fuel Processing Technology, 18 (1988) 185-199.
8. Garrett, D.E., CHEMICAL ENGINEERING ECONOMICS, Van Nostrand
    Reinhold, 1989.
9. CAMERON HYDRAULIC DATA, Ingersoll-Rand, 16'th Edition, 1984.
10. Santos, J.D., "Coal Gasification and Methanol Production,"
    paper presented at Symposium on Energy Production Processes
    for the Institution of Chemical Engineers, London, England,
    April, 1988.