American Institute of Chemical Engineers

AIChE®

2007 National Student Design Competition

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

Professor Richard L. Long

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

AIChE

October 2006

Dear Chemical Engineering Department Heads and Student Chapter Advisors,

I am pleased to send you the 2007 AIChE National Student Design Competition statement. Please forward it to those faculty teaching design courses. Following is this year's challenge:

"Separation Technology Evaluation for Economic Recovery of Pyridine."

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, 2007.

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 Wednesday, June 6, 2007. Please maintain a copy for your files. To order additional copies of the Student Design Competition statement, email awards@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 awards@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
2007

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, 2007. 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, 2007.**

AIChE National Student Design Competition - 2007

Separation Technology Evaluation for Economic Recovery of Pyridine

1.0 Introduction and Scope

The pyridine manufacturing process consists of a vapor phase catalyzed reaction and purification processes. Pyridine and 3-methylpyridine are synthetically co-produced in a circulating fluidized bed reactor. Impurities are also produced in the reaction process. These impurities are removed based on customer needs. During separation processes to make finished goods, useful product is lost to various streams and must be recovered. The subject of this project is to recover the pyridine and 3-methylpyridine from an impurity stream for recycle back to the process at the lowest processing cost that meets targeted capital payback criteria.

You are the design engineer from an engineering consulting firm that has been hired to evaluate potential separation technologies and make a recommendation on the most cost effective new process for recovery of pyridine and 3-methylpyridine from this stream. The design must meet the specified criteria for waste disposal, minimal product losses, and capital payback requirement.

2.0 General Process Description

A stream containing light boiling impurities, water, pyridine and 3–methylpyridine are processed to remove the light boiling impurities through separation technologies. The current process generates recycle streams that need further processing. Current operating costs for recovering pyridine from these streams is $0.04/lb of recycle (pyridine + 3-methylpyridine + water + light boiling impurities), approximately $800,000 per year.

An energy efficient, low capital means of recovering the pyridine and 3-methylpyridine from water and the light boiling impurities is preferred.

3.0 Alternatives to Be Considered

Pyridine and 3-methylpyridine must be separated from water and light impurities. This is complicated by azeotropes of the organic components with water (pyridine, 3-methylpyridine and the light boiling impurities azeotrope with water). Potential alternatives to be considered but not limited to are shown below:

Removal of water followed by separation of light impurities from products

3.0.1 Chemical treatment of water + lights + pyridine stream with caustic to form two layers, layer separation of organics, followed by separation of light impurities from pyridine

3.0.2 Removal of water using membrane technology, followed by separation of light impurities from pyridine

3.0.3 Adsorption of water on molecular sieves, followed by separation of light impurities from pyridine

4.0 Design Keys

4.0.1 Composition of Stream Requiring Pyridine and 3-Methylpyridine Recovery

Components	MW	Flows lb/hr	Weight %
METHANOL	32.04	130	5%
ACETONITRILE	41.05	312	12%
PYRIDINE	79.1	780	30%
3-METHYLPYRIDINE	93.13	208	8%
n-BUTYRONITRILE	69.11	26	1%
XYLENE (o,m, & p)	106.17	26	1%
WATER	18.02	1118	43%
Total		2600	100%

4.0.2 Equipment Sizing Basis
Equipment should be sized for the specified stream requiring pyridine and 3-methylpyridine recovery + 20% contingency to allow for maintenance downtime.

4.0.3 Utilities
The following utilities are available at the manufacturing site within 200 ft of where the proposed pyridine recovery process will be installed:
Steam = 180 psig pressure, 380 ºF saturated steam temperature
Cooling water = 85 ºF supply temperature, maximum 120 ºF return temperature, 40 psig pressure
Nitrogen = > 98% purity, 100 psig pressure
Plant and instrument air = 80 ºF temperature, 100 psig pressure, dew point = -22 ºF
City water =40 psig pressure, 55-65 ºF temperature
Purified water (boiler feed water quality) = 200 ºF temp, 40 psig pressure
Electric Power = 480 V, 3 phase, 60 Hz
Natural gas = 30 psig pressure

4.0.4 Process Conditions and Constraints
The process is to be designed with sufficient automation that additional operating personnel will not be required. A Distributed Control System is available for controlling the process instrumentation. A continuous process is preferred for ease of operations. Tanks are available in the area where the new process equipment will be installed within

200 ft for storage of the stream requiring pyridine and 3-methylpyridine recovery, recovered pyridine stream, recovered 3-methylpyridine, and waste streams.

4.0.5 Heat Generation and Removal
Heat input could be provided through electrical heating, steam, or a natural gas fired furnace with circulating heat transfer oil. Cooling could be provided through air cooled exchangers or cooling water cooled exchangers.

4.0.6 Waste Water Processing Capabilities
Water with organic concentrations up to a maximum of 1% and a pH of 4-12 can be processed on-site at the facilities waste water treatment plant for removal of organics and pH adjustment. If the new process generates waste water with > 1% organics, a pH < 4 or pH >12, it must be sent off site for treatment at $4.00/gal.

4.0.7 Liquid Waste Fuel Processing Capabilities
Liquid organic waste streams must be < 5% pyridine and < 15% water in order to be used on-site as fuel to be equivalent with the existing process. If the liquid organic waste stream is > 15% water, it must be sent off site for disposal at a cost of $0.20/lb.

5.0 Environmental/Health/Safety

The proposed design must comply with U.S. environmental laws and protect the safety and health of the manufacturing site personnel and the community. All equipment should be designed per good engineering practice and meet or exceed applicable U.S. codes and standards.

6.0 Quality Requirements

The recovered pyridine and 3-methylpyridine streams from the new process must be capable of being purified to meet finished goods specifications. The recovered material from the new process would have to be incorporated into one of the following streams based on its quality as specified. The additional processing costs for these streams are included below:

6.0.1 Pyridine Finished Goods Quality Specifications:

Pyridine	99.75% minimum
3-Methylpyridine	0.01% maximum
N-butyronitrile	0.05% maximum
Water	0.1% maximum

No additional processing necessary

6.0.2 3-Methylpyridine Finished Goods Quality Specifications:

3-Methylpyridine	98.0% minimum
Sum of light boiling impurities	0.2% maximum

Water	0.2% maximum

No additional processing necessary

6.0.3 Crude Quality Specifications:

Pyridine and 3-Methylpyridine	98.0% minimum
N-butyronitrile	0.03% maximum
Xylene	0.1% maximum
Water	1.0 % maximum

Additional processing energy cost = $0.07/lb of crude

6.0.4 Pyridine Intermediate Quality Specifications:

Pyridine	98.0% minimum
3-Methylpyridine	1.0% maximum
N-butyronitrile	0.04% maximum
Xylene	0.1% maximum
Water	1.0% maximum

Additional processing energy cost = $0.04/lb of pyridine intermediate cut

6.0.5 3-Methylpyridine Intermediate Quality Specifications:

3-Methylpyridine	98.0% minimum
Pyridine	1.0% maximum
N-butyronitrile	0.04% maximum
Xylene	0.1% maximum
Water	1.0% maximum

Additional processing energy cost = $0.04/lb of 3-methylpyridine intermediate cut

7.0 Cost Data

	$/Unit	Unit
Nat gas	11.00	MCF(Std)
Electricity	35.00	KWH
City Water	1.00	MGAL
Steam	17.00	MLB
Nitrogen	2.25	MCF(Std)
50% Caustic	0.125	LB

Additional cost data can be found in Plant Design and Economics for Chemical Engineers, Peters and Timmerhaus, 5th edition, McGraw-Hill, 2003.

Capital investment must meet a 3 year payback criteria.

8.0 Physical Property Data

Vapor Pressure Data

Temperature in ºC for the indicated pressure.

Compound	Acetonitrile	N-butyronitrile	Methanol	3-Methylpyridine	Pyridine	M-xylene	Water
Chemical Formula	C2H3N	C4H7N	CH4O	C6H7N	C5H5N	C8H10	H2O
Molecular Weight	41.05	69.11	32.04	93.13	79.1	106.17	18.02
1 kPa	-20 e	8 e	-20.4	28.8	8 e	23.4	7.0
10 kPa	21.4	52.3	15.2	75.2	51.0	69.8	45.8
100 kPa	81.2	117.2	64.2	143.7	114.9	138.7	99.6

e – indicates an extrapolation

Compound	Acetonitrile	N-butyronitrile	Methanol	3-Methylpyridine	Pyridine	Xylene	Water
Chemical Formula	C2H3N	C4H7N	CH4O	C6H7N	C5H5N	C8H10	H2O
Molecular Weight	41.05	69.11	32.04	93.13	79.1	106.17	18.02
CAS registry number	75-05-8	109-74-0	67-56-1	108-99-6	110-86-1	108-38-3	7732-18-5
Specific gravity of liquid at 20 º C	0.783	0.7936	0.792	0.961	0.982	0.867	1.000
Viscosity of liquid in mPas at 25 º C	0.369	0.553	0.544	0.87	0.879	0.603	0.89
Thermal conductivity of liquid in W/m K at 25 º C	0.188		0.200	0.140	0.165	0.130	0.607
Specific heat of liquid in cal/g º C	0.541 at 21-76 C	0.547 at 21-113 C	0.601 at 15-20 C	0.4073	0.431 at 21-108 C	0.397 at 30 C	1.0 at 30 C
Normal Boiling point (º C)	81.6	117.6	64.7	143.5	115.4	139.3	100.0
Heat of vaporization in cal/g	173.68 at 80 º C	114.91 at 117.4 º C	262.79 at 64.7 º C	95.85 at 144 º C	107.36 at 114 º C	81.2 at 138.35 º C	539.83 at 100 º C
Dissociation constant with water at 25 º C (pKa)	-10	-10	15.2	5.68	5.25	41	15.74
Azeotrope (temperature and weight % water)	80.1 º C with 16.3% water	87.5 º C with 31% water	no azeotrope with water	96.7 º C with 63% water	93.6 º C with 41.3% water	94.5 º C with 40% water	N/A
Solubility in water at 10 º C	infinitely	slightly soluble	infinitely	infinitely	infinitely	insoluble	N/A

9.0 Reporting Requirements

The report format must adhere to the following outline:

A. Title page
B. Table of Contents
C. Executive Summary – One page summary of the report
D. Introduction – Restatement of the problem with background and objectives
E. Discussion – Present the alternative design options considered, evaluate the strengths and weaknesses of each alternative, list any special hazards associated with each design, and define the final design basis.
F. Summary – Summarize the results of the evaluation including the recommended design option, the operating cost, capital cost and payback.
G. Conclusions – Interpret the results of the evaluation. List your conclusions in decreasing order of significance.
H. Recommendations – State the recommended design for the process emphasizing the technical feasibility and optimum economics.
I. Project Assumptions – List key assumptions used for the design and economic analysis.
J. Process Flow Diagram – The PFD should include the major equipment with a stream number for each major process stream. Show the basic process control instrumentation including points of measurement for temperatures, pressures, flow rates, pH, and the associated control devices.
K. Mass and Energy Balance – Provide a mass and energy balance for the new process to recover pyridine and 3-methylpyridine from water and light boiling impurities. For each stream on the PFD, provide the stream number, stream description, composition by weight %, temperature, pressure and flow rate. Include a table with a summary of utility consumption.
L. Hazard and environmental analyses – Identify and quantify the waste streams. Specify the recommended means of waste processing or disposal. Summarize the key safety hazards of the process and the aspect of the design that mitigates/reduces the potential hazard.
M. Equipment summary – Provide a list of all equipment used in the process including a description, size of the equipment, and material of construction.
N. Economic analysis – Provide a summary of the payback on the capital investment including the operating cost for the new process and capital estimate for the installed equipment.
O. Engineering calculations – Include all pertinent hand calculations.
P. Computer programs – Include input and output files and an explanation of the model used including nomenclature.
Q. Computer process simulations – Include input and output files and a simulator flow chart for the optimum set of conditions for any process simulation using standard process simulator programs. Provide an explanation of the model used including nomenclature.

10.0 Websites of Interest:

http://kekule.chem.csus.edu/forkey/Extraction/Forkeys_extraction.html
http://en.wikipedia.org/wiki/Pyridine
http://en.wikipedia.org/wiki/PH
http://www.sigmaaldrich.com/Brands/Aldrich/Tech_Bulletins/AL_143/Molecular_Sieves.html
http://www.gracedavison.com/eusilica/Adsorbents/product/zeolite_molecular_sieve.htm
http:/www.iupac.org/publications/pac/1995/pdf/6706x0993.pdf

http://www.sulzerchemtech.com/eprise/SulzerChemtech/Sites/products_services/pervap.html
http://www.cheresources.com/pervaporation.shtml

11.0 References

Perry's Chemical Engineers Handbook 6th Edition, McGraw Hill, 1984.

Linde, David R., Handbook of Chemistry and Physics 77th Edition, CRC Press Incorporated, 1996.

Linde, David R., Handbook of Chemistry and Physics 82nd Edition, CRC Press Incorporated, 2001

Horsley, Lee H., Azeotropic Data III, Advances in Chemistry Series, American Chemical Society, 1987