1997 Student Design Competition

If there are any questions about the design problem, 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 NATIONAL STUDENT DESIGN COMPETITION 1997

Benzene Alkylation Fractionation Process Unit Revamp

DEADLINE FOR MAILING:

Solutions must be postmarked no later than midnight, June 6, 1997.

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 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 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. Judging, however, will be based on the overall suitability of the solutions, not on skills in manipulating computer programs.

The 1997 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. Solution 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 6, 1997. 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 no 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 6, 1997.
- The finished report must 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 not be used.

SENDING THE SOLUTION TO AICHE

- Two copies of each of the solution(s) must be sent to the address below; 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 <u>midnight</u>, June 6, 1997. 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 6, 1997

Benzene Alkylation Fractionation Process Unit Revamp

I. OBJECTIVE AND SCOPE

1. Determine the optimum fractionation process flow scheme based on installed cost of new equipment and variable operating costs, while utilizing certain specified existing fractionation columns, for the revamp of a Cumene Process Unit. The optimization should include but is not limited to raw material utilization, product and by-product credits, utility costs and credits, and capital investments for any new equipment. The optimization is to be performed using a value of 15% for the cost of capital (minimum acceptable return), and should be based upon after-tax discounted cash flow techniques and a plant service life of 10 years.

Refer to Sketch No. 1 (page 14) for a typical flow scheme for a new unit, and to Sketch No. 2 (page 15) for the scope of the revamp work.

All results and supporting calculations shall be submitted in English units.

- 2. The following should be provided with the solution in the format specified:
- A. Title Page
- B. Table of Contents
- C. Executive Summary Two (2) page condensation of the report
- D. Introduction Restatement of the problem at hand, covering background and objectives.
- E. Data, Calculations, and Results Provide a table showing for each case considered the parameters that were evaluated, the procedure used to do the evaluation, input data, the source of the data for the evaluation, and the results of each case evaluated.
- F. Summary Provide a descriptive summary of the various cases considered in E above, the results, and conclusions arrived at and the rationale behind it.
- G. Optimum Case Provide a detailed description of the selected case which should include a description of the process flow scheme, the function of each major equipment and their connectivity to each other, feed injection and product withdrawal points, cost-saving features, energy recovery features, and other special design features.

1

- H. Equipment Summary Report for the Optimum Case Provide a list of all the equipment used in the process. Include suitability assessment of the existing equipment, and equipment type and description, operating conditions, sizes, duties, and other important specifications. Include costs (equipment cost and installed cost) of new equipment.
- I. Utilities Summary for the Optimum Case Provide table showing for each utility user the equipment duty, utility consumption, and the specific utility cost. Show also the total consumption and cost for each utility category.
- J. Process Flow Diagram (PFD) Show the optimized flow scheme with all the major process equipment, and with a stream number designated for each of the major process streams. Show also the basic process control instrumentation, i.e. point of measurement for temperatures, pressures, and flow rates and the associated control device.
- K. Mass and Heat Balance Provide a mass and heat balance summary which includes heat input or removal duties; and report in flow sequence for each corresponding stream on the PFD its stream number, description, temperature, pressure, volumetric flow (in gpm for liquids, cfs for vapors), molecular wt., mols/hr, lbs/hr and heat content in 10⁶ Btu/hr.
- L. Stream Compositions Provide composition in lb-mols/hr of all the streams entering and leaving the section battery limits and also the feeds and net product streams from each fractionation section. Show also the impurities of the cumene product streams in wppm units.
- M. Computer Process Simulators and Other Programs Use of the generally accepted process simulators (e.g. Aspen, Hysim, Sim-Sci, Chemcad, etc.) together with spreadsheets or personally-developed computer programs are acceptable.
- N. Back-up Data and Calculations Provide documentation for all hand calculations. Include flow charts, input files and output reports (edited and condensed) from computer programs associated with the optimized case only. Input and results for preliminary cases should be included in the tabulation of data and results described in E above. Provide an explanation of the computer model(s) used and also the nomenclature and relevant information to familiarize the reader with the capability and acceptability of the computer program utilized. Provide explanations of assumptions made and details not included elsewhere in the report.

II. PROCESS DESCRIPTION AND DESIGN CONSIDERATIONS

Cumene is produced by reacting propylene and benzene under controlled conditions according to the following reaction:

Propylene + Benzene = Cumene + Di-isopropylbenzene (DIPB)+ Other Alkylation By-Products

The propylene feed normally contains propane and small amounts of light hydrocarbons typically ranging from C2's thru C4's. Other light alkenes present in the propylene feed will react with benzene and form the corresponding alkylbenzene product. The non-reactive light saturates in the feed will leave with the alkylation reactor effluent and are normally removed at the overhead of a downstream depropanizer.

The unreacted benzene from the alkylation reactor is typically recovered as a recycle stream in the downstream fractionation section where it is pumped back to the alkylation and the transalkylation zones. A second recycle stream, consisting mainly of DIPB, is also recycled and fed together with recycle benzene to the Trans-alkylation reactor in order to redistribute the propyl radical, thus:

Di-isopropylbenzene + Benzene = Cumene + Trans-alkylation By-Products

Aside from recovering the recycle material, the Fractionation section also yields the net cumene product stream and a "heavies" stream which consists mostly of the small amounts of heavier poly-alkylbenzene by-products formed in the process.

III. UNIT CAPACITY

Cumene Production = 120,200 lbs/Hr

IV. FEED SPECIFICATIONS

Fresh Benzene Feed Composition, mol%:

Component:	<u>mol%</u>
Water	0.1000
Methyl Cyclopentane	0.1157
Benzene	99.7513
Methyl Cyclohexane	0.0203
Toluene	0.0127
Total	100.0000

Fresh Propylene Feed Composition, mol%:

Water	0.0120
Ethane	0.3096
Propylene	68.6147
Propane	31.0408
Butylene	0.0020
Isobutane	_0.0209
Total	100.0000

V. PRODUCT SPECIFICATIONS

Cumene Product:

Cumene Purity, wt%	99.97	minimum
Butylbenzenes, wppm	40	maximum
Toluenes, wppm	15	maximum
Cymenes, wppm	10	maximum
Benzene and Non-Aromatics, wppm	10	maximum
Others, wppm	225	maximum

Propane Product:

The process kinetics are not affected by the presence of light saturated paraffin hydrocarbons, such as butane, propane, or ethane, but it is best to limit the build-up of these components in the recycle loop in order to avoid unnecessary increase in utilities and equipment costs. Depending on the economics, the butanes and lighter saturates (essentially propane) that are present in the propylene feed may be recovered at the depropanizer overhead, either as a vapor stream and valued as fuel gas, or as a liquid stream and valued as LPG. In any case, the aromatics content of the product stream should not exceed 0.01 wt%.

Heavies:

The heavies recovered as net bottoms from the Di-isopropylbenzene (DIPB) Column should contain a maximum of 5% of the intermediate product DIPB and lighter. For the purpose of this optimization, this by-product stream will be valued as fuel oil.

VI. OPERATING AND BATTERY LIMITS STREAM CONDITIONS

- 1. The design engineer will determine the optimum operating conditions (e.g. reflux rates for each column, and pressures, temperatures, and flow rates for the intermediate streams) in the fractionation section.
- 2. The propylene feed will be delivered as a liquid stream at 100 °F, at sufficient pressure to get into the reactor section. The benzene feed is available at 100 °F from atmospheric storage.
- 3. All liquid product streams will be cooled to a minimum of 100 °F and delivered at battery limits at a pressure of at least 25 psi above its vapor pressure or at 50 psig, whichever is greater.
- 4. The total combined feed stream to the Alkylation Reaction Section is controlled at 280 °F. Allow a maximum of 60 psi pressure drop across this section. Assume the temperature of the stream returning to the Fractionation section from the Alkylation reaction section to be 302 °F, and the stream pressure controlled at 375 psig.
- 5. The total combined feed stream to the Trans-alkylation Reaction Section is controlled at 320 °F. Allow a maximum of 20 psi pressure drop across this section. Assume the temperature of the stream returning to the Fractionation section from the Trans-alkylation Reaction Section to be 320 °F, and the stream pressure controlled at 210 psig.

VII. REACTION YIELDS

The following are the estimated wt. % yields for the alkylation reactor and the corresponding trans-alkylation reactor yields, based on a given amount of pure propylene charge:

Component:	Alkylation Wt. %	Trans-alkylation Wt. %
Propylene	-100.0000 - 0.0039	000.0000
Butylene Benzene	-168.1835	-16.3570
Toluene Cumene	- 0.0214 232.7018	50.7652
n-Propylbenzene p-Cymene	0.0346 0.0306	0.0087 - 0.0025
t-Butylbenzene m-Di-isopropylbenzene	0.0080 20.3314	- 0.0007 -20.2323
p -Di-isopropylbenzene Alkylation Heavies *	14.7797 0.3227	-14.4935
Trans-alkylation Heavies * Total	<u>0.0000</u> 000.0000	$\frac{0.3121}{000.0000}$

^{*} Non-Standard Components Properties are shown below:

Normal Boiling Pt. <u>°F</u>	API <u>Gravity</u>	Lb./Gal.	UOP K Factor
533.83 502.25	1.375 19.72	8.868 7.791	10.3 [^] 10.57
	<u>°F</u> 533.83	<u>or</u> <u>Gravity</u> 533.83 1.375	<u>Gravity</u> 533.83 1.375 8.868

Note: Negative values indicate component is consumed, otherwise the component is produced in the process.

VIII. PROCESS DESIGN GUIDELINES

- 1. Assume complete conversion of alkenes in the alkylation reactor, i.e. no residual alkenes in the reactor effluent stream.
- 2. Assume that only 50% of the Di-isopropylbenzenes are converted each pass through the transalkylation reactor.
- 3. In order to avoid excessive formation of poly-alkylated by-products, which translates to yield loss, the reaction environment for both the alkylation and the trans-alkylation reaction are maintained under a relatively high concentrations of the phenyl (C6H6-) group as compared to the propyl (-C3H5) group. For this design, a minimum benzene-to-propylene molar ratio of 4.0 has to be maintained in the reactants stream to the alkylation reactor, and also a 4.0 molar ratio of benzene-to-DIPB in the reactants stream to the trans-alkylation reactor.
- 4. For obvious reasons, the concentration of cumene in the recycle stream should also be minimized and kept below 1.3 mol% in the charge to each reactors.
- 5. While the alkylation reactor is able to tolerate the presence of moisture, the trans-alkylation reactor is best when operating dry, thus the benzene to this section should be stripped of its moisture content.
- 6. For design purposes, the recycle benzene column overhead should have at least 90 mol% benzene purity. (In order to meet this requirement, it may be necessary to maintain a drag stream withdrawal at strategic locations in the unit in order to prevent build-up of hard-to-fractionate components such as the light aromatics. (See Item 8 below for evaluating the commercial value of the drag stream.)
- 7. The design engineer may specify other drag streams in order to prevent excessive buildup of other impurities in the system as deemed appropriate to meet product purity specifications.
- 8. For optimization purposes, the value assigned to any drag stream may be taken as: 0.75 (wt. Bz) (Cost of Bz per unit wt.) + 0.5 (wt. Cumene) (Cost of cumene per unit wt.)
- 9. Use water cooling only (as opposed to air cooling) when waste heat is not suitable for recovery. Cooling water is available at 85 °F. Maximum allowable temperature rise is 18 °F.

10. Below are design guidelines for setting up the hydraulics of the process unit:

Atmospheric Pressure:

14.7

psia

The design pressure for new equipment should be at least 50 psig and should be a minimum of 25 psi above its maximum operating pressure.

Assume centrifugal pumps shutoff pressure is equal to suction pressure \pm 115% of pump design head.

Maximum Allowable Pressure Drops, psi:*

Column trays	0.125	psi per theoretical stage; rounded to the next higher whole psi value.
Process heat exchangers & coolers	10. 5.	psi (if all liquid) psi (if all vapor)
Column Ovhd Condensers and piping and instrumentation from column to receiver	7.	psi
Thermosyphon reboiler effluent piping	0.1	psi
Control Valves	25.	psi

^{*} Assume piping pressure drop has been included in the allowance for the equipment pressure drop.

IX. UTILIZATION OF EXISTING EQUIPMENT

Existing fractionation columns from a Cumene unit based on a different process are available, and may be used for the new unit. It has been confirmed that the carbon steel columns are suitable for the requirements of the new process, from a mechanical and metallurgical standpoint.

The following are the descriptions of the existing columns, which are currently equipped with valve trays:

Previous Service:	Design Temp. ${}^{\circ}\underline{F}$	Design Pres. Psig	Inside Dia. Feet-Inches	No.of Ideal Trays
Benzene Recycle	550	100 & Full Vacuum	10 - 6	35
Cumene Column	580	100 & Full Vacuum	6 - 6	48
De-Propanizer	500	300	4 - 0	18

Notes:

1. If existing columns are bottlenecked, design engineer may add additional columns and the necessary auxiliary equipment or completely replace the existing Fractionating system in order to de-bottleneck the unit.

X. COST OF RAW MATERIALS, PRODUCTS, AND UTILITIES

Cost of Raw Materials and Products:

Propylene	\$ 0.14	per Lb.
Benzene	0.11	per Lb.
Cumene	0.21	per Lb.
LPG	0.07	per Lb.

Cost of Utilities:

Fuel Oil \$ 2.28 per million Btu of net heating value
Fuel Gas 2.00 per million Btu of net heating value

0.10 per 1000 gallops

Cooling Water 0.10 per 1000 gallons

Boiler Feed Water Utilize steam condensate available at 212 °F;

assume available at no cost for steam generating

equipment inside process battery limits.

Electricity \$ 0.06 per KWH

Steam (Saturated Conditions):

 610.3 psig
 \$ 3.30 per 1000 Lb.

 250.3 psig
 3.00 per 1000 Lb.

 50.3 psig
 2.50 per 1000 Lb.

 19.3 psig
 2.40 per 1000 Lb.

Circulating hot oil is available as a heating medium for higher temperature service, but supply is limited to a maximum of 15.0 million Btu per hour.

Cost of hot oil utility = \$ 5.00 per million Btu; Supply temperature = 600 °F;

Supply Pressure = 60 psig; Sp. heat = 0.627 Btu/Lb-°F; Ave. Flowing Sp. Gr. = 0.847

Note: Assume buy back prices for utilities generated in the process from by-products or as a result of heat recovery are the same as cost of importing them from outside battery limits.

XI. EQUIPMENT SIZING GUIDELINES

1. Assume that as long as the existing column trays are adequate for the new service, the overhead receivers will likewise be suitable, and that retraying of the existing columns will not be required. New reboilers, condensers, exchangers, and pumps will have to be installed for all the existing columns. The expense for installing new inlet or outlet nozzles for an existing vessel may also be ignored.

- 2. Overhead receivers shall be sized based on a minimum 5 minutes residence time at 50% full, based on total liquid rate. Design diameters and tangent lengths to the nearest 6-inch dimension.
- 3. New columns should not be less than 2'-6" in diameter and shall be designed using sieve trays. Column diameters shall be determined using any commercially acceptable tray sizing procedure, e.g. FRI, Glitsch, Koch, Nutter, etc. The procedure used should be identified and the calculations documented as necessary.
- 4. Assume 24" tray spacing for both new and existing columns. For cost estimating purposes, assume 75% tray efficiency for all columns. A maximum jet flooding of 95% will be acceptable for existing columns, but new columns shall be designed for a maximum of 85% jet flood.
- 5. Steam generators if utilized for heat recovery should have a minimum approach temperature of 25 °F (hot side outlet cold side outlet).
- 6. The following overall heat transfer coefficients shall be used for determining heat exchange surface requirement for heat exchangers:

Type of Exchanger	Type of Exchanger Tube Fluid	
		Btu/hr-sq. ft°F
Light Hydrocarbon Condenser	Cooling water	100
Steam Reboilers	Steam	120
Oil - Oil Exchanger	Oil	75
Oil - Water Cooler	Water	80
Steam Generators	Condensing Hydrocarbons	110
Steam Heaters	Condensing Steam	100
Hot Oil Reboilers	Hot Oil	70

- 7. Each process pump shall have a standby 100% spare. Rated flow for each shall be 100% of normal flow. Design pump motor HP for 120% of normal design flow requirement. Use the efficiencies of centrifugal pumps and motors as determined from Figures 37 and 38 respectively on pages 520-521 of Peters and Timmerhaus, **Plant Design and Economics for Chemical Engineers**, 4th Ed., McGraw-Hill, 1991. Assume overall pump efficiency of 70% for reciprocating pumps.
- 8. Column reboilers shall be designed for a maximum of 33 wt% vaporization.

XII. ECONOMIC ANALYSIS GUIDELINES

- 1. Estimate purchased equipment costs using the correlations provided in Table XII-A below. Costs for equipment not shown may be estimated from Peters & Timmerhaus, **Plant Design and Economics for Chemical Engineers**, 4th Edition, McGraw-Hill, 1991, or from process simulators or any other generally acceptable and properly documented sources.
- 2. Projected capital cost is to be estimated using method C, p.180 of Peters & Timmerhaus.

Table XII-A: PURCHASED EQUIPMENT COST CORRELATIONS

Note: The equipment cost correlations shown yield costs for the 2nd quarter of 1996. Adjustments to current costs should be based on the **Oil & Gas Journal**, "Nelson-Farrar Quarterly Costimating, Itemized Refining Cost Indexes for Equipment or Materials."

A. VESSELS: $$=Wt \times Cf$ $Wt = (V_1 \times 10.7)$

 $Wt = (V_1 \times 10.7 \times V_t \times V_d) + (2(D^2 \times 1.085) \times V_t \times 40.8)$

Cf = 4.5, if Wt < 2000 lbs.

= 2.0 + 5000/Wt, if Wt < 5000 lbs. = 1.5 + 7500/Wt, if Wt < 10,000 lbs.

= 1.625 + 6250/Wt, if Wt < 50,000 lbs.

= 1.5 + 12500/Wt, if otherwise

where:

Wt = Vessel weight, pounds

Cf = Cost factor

 V_1 = vessel tangent length, feet V_t = vessel thickness, inches V_d = vessel diameter, inches

D = vessel diameter, feet

B. TRAYS:

Tray = 100 D Fn

Fn = 2.9, if Nt < 5

= 0.5 + 10/Nt, if Nt = 5 - 20

= 1.0, if Nt = >20

where:

D = tray diameter, feet

Fn = Factor for tray quantity

Nt = No. of actual trays

C. HEAT EXCHANGERS:

$$$ = ($40 \times Sa) + $2000, \text{ if } 50 - 500 \text{ ft}^2$$

= (\$13.334 x Sa) + \$15333, \text{ if } 501 - 2000 \text{ ft}^2
= (\$10 x Sa) + \$22,000, \text{ if } 2001 - 10,000 \text{ ft}^2

where:

Sa = Exchanger surface area, ft²

D. PUMPS:

API Centrifugal Pumps:

where:

BHP = Brake Horse Power

API Proportioning Pumps:

 $= (HHP \times \$300) + \$1,000$

where:

HHP = Hydraulic Horse Power

E. ELECTRIC MOTORS:

$$$ = ($100 x HP) + $100, if \le 5 HP$$
= (\$80 x HP) + \$200, if 7 1/2 - 50 HP
= (\$75 x HP) + \$600, if 60 - 200 HP
= (\$100 x HP) + \$5,000, if > 200 HP

where:

HP = Name Plate Horse Power

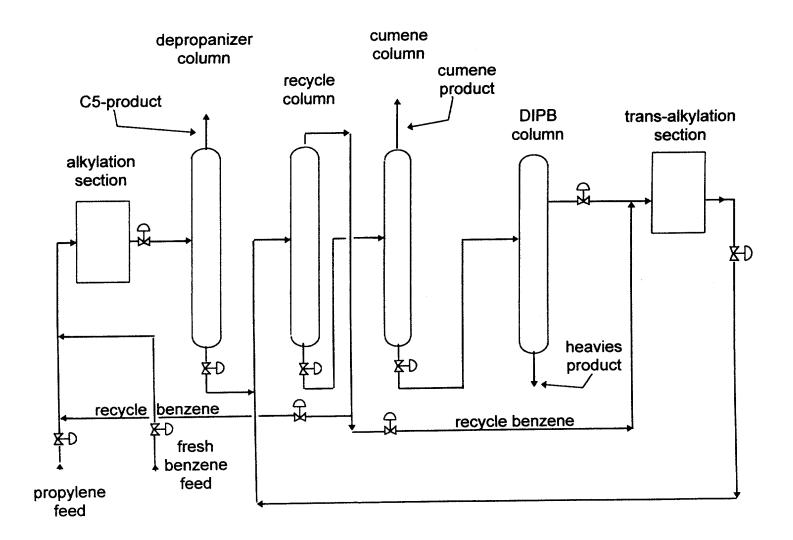
F. MISCELLANEOUS EQUIPMENT:

Vacuum Ejector, Continuous Service:

Single Stage, steam powered ejector = \$1,200 Two Stage, steam powered ejector = \$3,000

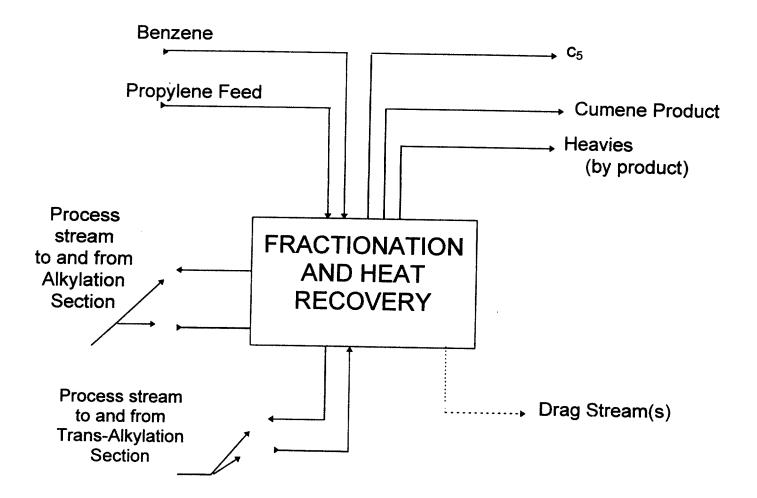
Single Stage = 27" Hg. vacuum, with 275 Lb/Hr of 250 psig steam required. Two Stage = 29" Hg. vacuum, with 730 Lb/Hr of 250 psig steam required.

Sketch No. 1
A typical flow scheme for a new unit may be as follows:



Sketch No. 2 Scope of Design

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