



**American
Institute of Chemical Engineers**

STUDENT CONTEST PROBLEM

1986

1986 CONTEST PROBLEM

AMERICAN INSTITUTE OF CHEMICAL ENGINEERS STUDENT CHAPTERS

Open Only to Undergraduates or Those
Without a Degree in Chemical Engineering

DEADLINE FOR MAILING

Solution must be postmarked not later than midnight, June 1, 1986

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 readily available in handbooks and similar reference works. The use of textbooks, handbooks, journal articles, and lecture notes is permitted. In cases where there is disagreement in the data reported in the literature, the values given in the problem have been chosen as being most nearly applicable.

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 solution, not on skills in manipulating computer programs.

The Student Contest Problem is designed to be solved by individual chemical engineering students working entirely alone, and it is judged on that basis. There are, however, other academically sound approaches to using the problem. The following confidentiality rules therefore apply:

1. *For students 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 solution. Discussion with faculty and students at that school is permitted only after complete final reports have been submitted to the chapter counselor.
2. *For students whose solutions are not intended for the contest:* Discussion with faculty and with other students at that school 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 schools, or with individuals in the same school who are still working on the problem for the contest, until after June 1, 1986. 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 these conditions.

A period of not more than thirty consecutive days is allowed for completion of the solution. This period may be selected at the discretion of the individual counselor, but in order to be eligible for an award a solution must be postmarked not later than midnight, June 1, 1986.

The finished report should be submitted to the chapter counselor within the thirty-day period. There should not be any variation in form or content between the solution submitted to the chapter counselor and that sent to the AIChE office. The report should be neat and legible, but no part need be typewritten.

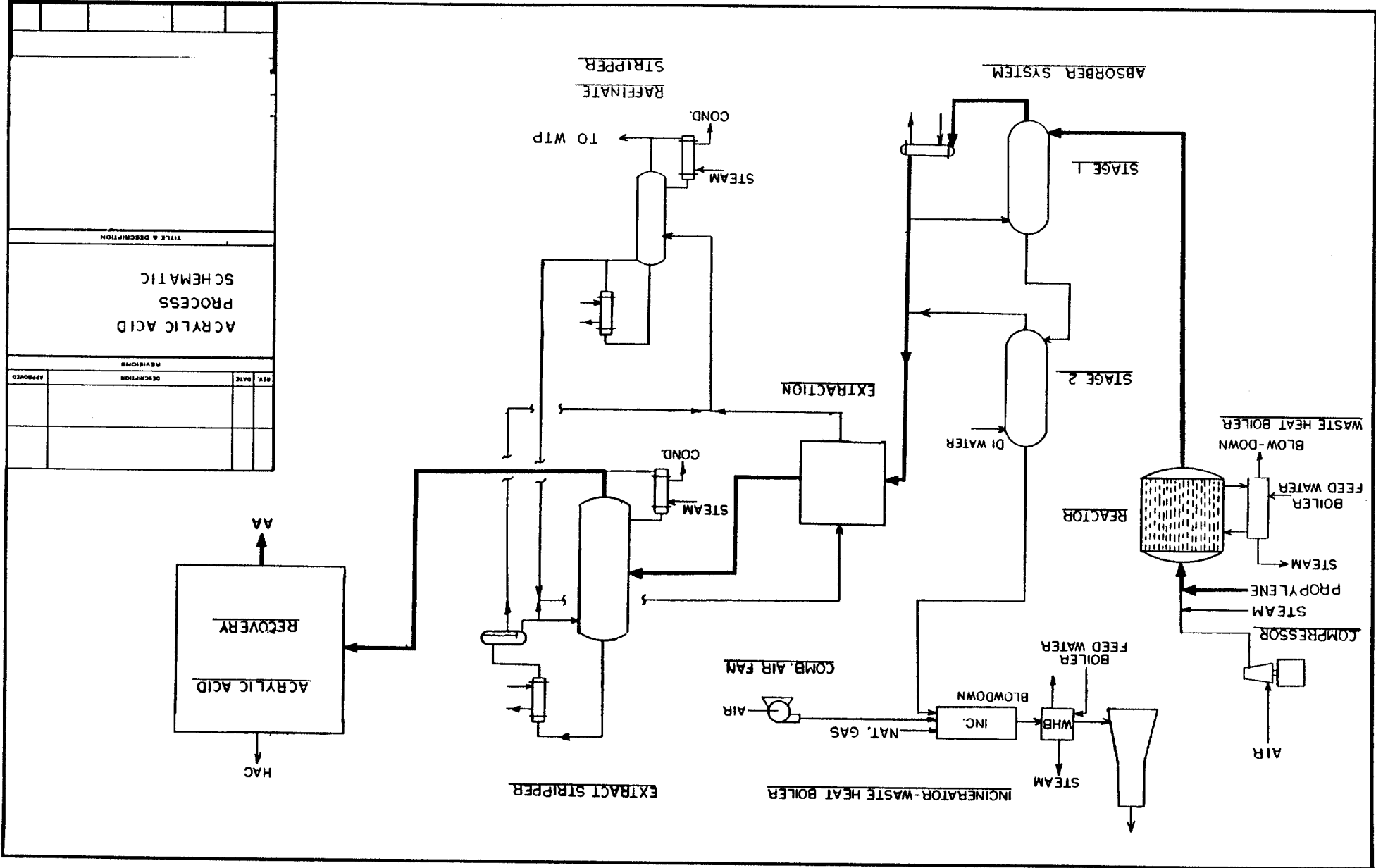
The solution should be accompanied by a letter of transmittal giving only the contestant's name, school address, home address, and student chapter, lightly attached to the report. This letter will be retained for identification by the Secretary of the Institute. The solution itself must bear no reference to the student's name or institution by which it might be identified. In this connection, graph paper bearing the name of the institution should be avoided.

Each counselor should select the best solution or solutions, not to exceed two, from his chapter and send these by registered mail to:

J.C. Forman, Executive Director and Secretary
American Institute of Chemical Engineers
345 East 47 Street
New York, New York 10017

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AICHE STUDENT CONTEST PROBLEM
1986
Production of Crude Acrylic Acid from Propylene

INTRODUCTION

Projected demands for acrylic acid over the next ten years indicate that a new production facility must be built and on stream in 1987. Acrylic acid (AA) is produced via air oxidation of propylene and is purified via solvent extraction and distillation to remove water and by-product acetic acid (HAc). An existing plant is already in operation using this basic technology, but the Research Department has developed some alternative extraction solvents that must be considered and there is a common belief that the purification section distillation system in the new facility can be more efficiently designed. In addition, a new catalyst has been developed which will allow us to consolidate the two-stage reactor system into a single reactor.

The by-product acetic acid can be sold for several uses in the industry. The waste water for the process can be handled in the existing waste treatment plant. The waste gas must be burned to meet environmental regulations. It is necessary, therefore, to develop a basic design of the new plant, determine the capital investment and operating costs, and then determine the manufacturing costs for comparison to the existing plant.

STATEMENT OF THE PROBLEM

Your objectives are:

1. Determine the oxidation reactor operating conditions based on information supplied by Research. Determine the size of the reactor and the size of the associated waste heat boilers.

2. Design the absorber to meet the recovery requirements specified.
3. Determine the heat and material balance for the incinerator based on the data supplied. Also determine the steam production.
4. Evaluate the two solvents that have been proposed for extracting the acrylic acid from the aqueous stream from the absorber. Laboratory data have been supplied for scale-up of the two columns in this section as it is very difficult to model this system.
5. Determine the optimum distillation column system to remove acetic acid from the acrylic acid.
6. Size and estimate the costs of the major pieces of equipment.
7. Estimate the capital investment based on the estimated purchase cost for the major equipment items.
8. Estimate the manufacturing costs.

The final report format should be as follows:

1. Cover letter to Mr. Jack Jones
2. Introduction: Concise problem statement
Background
Objectives
3. Conclusions
4. Recommendations for further work

Manufacturing Costs

It can be assumed that all investment will be in 1986. Production and 11yr. straight-line depreciation will start in 1987.

Raw Material Costs

Propylene	\$0.48/kg
By-product HAC credit	\$0.33/kg
Misc. Chemicals	\$0.04/kg of CAA

Utility Costs

Cooling water	\$ 0.020/K-liter
Deionized water	1.200/K-liter
Electricity	0.074/KW-hr
Natural gas	3.700/Million-kjoules
Refrigerated water	8.300/Million-kjoules
Steam(cost or credit)	20.000/K-kgrams
Boiler feed water	2.500/K-liter
((@ 50 deg C)	
Misc.*	0.033/kgram of AA produced

*This includes waste treatment, instrument air and electricity to operate pumps and other unlisted pieces of equipment.
(Note: K = thousands)

Other Costs

Labor, benefits, taxes, etc.	\$ 0.0147/\$investment/yr
Maintenance	0.04/\$investment/yr
Other support charges (Engr., Supplies, Admin., etc.)	0.0140/kggram of AA produced/yr

Cash Flow Information

Tax Rate	50%
Discount Rate	15%
Time	11 years
Ignore start-up costs	
Ignore inflation and investment tax credit	

References

1. W. Bauer, Jr. and F. T. Maher, *Encyclopedia of Chemical Processing and Design*, Vol. 1, Marcel Dekker, Inc., New York, New York, 1976, pp. 401-428.
2. Buford D. Smith, *Design of Equilibrium Stage Processes*, McGraw-Hill, New York, New York, 1963.
3. Robert E. Treybal, *Mass Transfer Operations*, McGraw-Hill, New York, New York, 1968.
4. H. R. C. Pratt, *Countercurrent Separation Processes*, Elsevier Publishing Company, New York, New York, 1967.

DESIGN DATA AND BASIS

(Including simplifying assumptions)

1. Material and Energy Balances

A complete heat and energy balance should be generated for the proposed process given the available data. It can be assumed that any steam generated will go into a plant header system and all steam used will come from this system. Credits and costs should be assigned accordingly.

A mass balance for the system should also be completed. Minor by-products have been ignored for this preliminary design as experience indicates they have no significant effect. Also, losses to vents and sampling may be ignored.

2. General Design Information/Guidelines

- a. In doing the various calculations, use the data supplied in the problem rather than data from other sources. NOTE: Some data may not agree with literature data. Use steam tables for water and steam.
- b. The plant should be designed as indicated by the flow-sheet and in the description. However, comments regarding the validity of the assumptions are expected as are comments, both qualitative and quantitative, on how the process might be improved. (i.e. energy efficiency, etc.)
- c. The design of each section may be scaled up or down linearly as required to cover minor discrepancies, + or - 5%.
- d. Cooling tower water is available at 30 deg C. Use a 10 deg C rise.
- e. Refrigerated water is available at 5 deg C. Use a 5 deg C rise.
- f. 5% of the water fed to a boiler for steam production is removed from the boiler as liquid to prevent the build-up of solids. The water fed to boilers is at 50 deg C.
- g. Vacuum systems will be required for some of the columns in this plant. Design of these systems need not be considered as part of the problem. The costs of the vacuum systems has been incorporated into the other cost factors.

3. General Distillation/Absorber Column Design Assumptions

- a. Assume sieve trays, except for the first absorber section, as the predominant information in the literature covers this type of tray.
- b. Assume 61cm (24 in) tray spacing.
- c. Pressure drop per tray = 3.5 mmHg.
- d. Use Figure 18-10 in Perry's 5th and 6th editions to determine the flood velocity for sieve tray calculations. Use Figure 18-39 to determine the flood velocity for a packed tower. Use 80% of flood as a maximum velocity. Use 25 dynes/cm for surface tension.
- e. Assume 50% tray efficiencies.
- f. Assume 80% active tray area.
- g. Assume 1 column diameter above the top tray and 2 column diameters below the bottom tray when calculating column length. Use the same criteria for above and below the packing where applicable.
- h. Use 550kPa steam for reboilers to minimize the tube wall temperature.
- i. Assume kinetic and potential energy and work terms are negligible when calculating the energy balances.

4. Oxidation Reactors/Absorber

Reactor

Propylene vapor is available at 600kPa @ 30 deg C. Air must be compressed to be fed to the Oxidation reactor. The power for this compressor will be supplied by an electric motor. Assume a turbine efficiency of 75% and a motor efficiency of 90%.

The optimum reactor size and the size of the waste heat boiler must be determined. For the reactor, assume:

tube I.D. = 45 mm
tube length = 4575 mm
Catalyst bulk density = 880 kg/cu. meter
(Assume each tube is completely filled with catalyst.)

The economic data and laboratory data required for this analysis has been supplied. It should be noted that while this reaction usually requires two reactors as discussed previously, a new catalyst has been developed that requires only one reactor, thus explaining the format of the data supplied.

For the feed, assume a molar ratio of O₂/C₃H₆ of 2.25 and a steam composition in the feed of 40 mole% to keep the reaction mixture from becoming too hot. Use 550kPa steam in the feed.

Steam generation from the reactor waste heat boiler should be at a pressure of 550 kPa.

To determine the acrylic acid production rate required from the Oxidation section, assume a 97% recovery of AA in the extraction and acrylic acid recovery sections. (Actual recovery may vary slightly depending on the final design of the plant.)

Absorber System

The absorber should be designed as a two section system to recover the AA from the vapor phase reactor effluent. The following assumptions should be made based on previous experience.

Stage 1 (Quench)

1. Use a packed column in which vapor is contacted with a large stream of cooled, recirculated condensate.
2. Assume that the condensate forms an ideal solution.
3. Assume an operating pressure of 760mmHg and neglect pressure drop for calculation purposes.
4. Assume that nitrogen, oxygen, carbon dioxide and propylene are insoluble in the liquid phase.
5. Assume that if the bed is packed to a depth of 40 feet with one inch Raschig rings, the vapor and liquid leaving this section are in equilibrium and are at 50 deg C.
6. Assume that the density and viscosity of the bottom solution equal that of water at the same temperature.
7. If the recycle condensate enters this section at 38 deg C, what is its rate and how large is the cooler?
8. Determine the diameter of this section using the conditions at the bottom of the column.

Stage 2 (Absorber)

1. In the second section, the AA is recovered by counter-current contact with water at 50 deg C.
2. A deionized water feed of 227 kgmoles/hr is used. (DI water is at 50 deg C.)
3. 99.9% recovery of AA in the reactor effluent is required.

Table 1. Physical Property Data

Component	Mole Wt.	Normal		Heat of Comb. ¹ Kcal/g-mole	Heat of Vap. ² cal/g-mole	Liquid Sp. Gr. Typ. Cond.
		Boil. Point Deg C	Melt. Point Deg C			
C ₃ H ₆	42.08	-47.4	-185.4	489.4	4697	—
CO ₂	44.01	—	—	—	NR	—
AA	72.06	141.6	13.0	317.2	7872	1.010
HAC	60.05	117.9	16.6	218.4	5733	0.973
O ₂	32.00	—	—	—	NR	—
N ₂	28.01	—	—	—	NR	—
H ₂ O	18.02	100.0	0.0	—	Use Steam Tables	—
CH ₄	16.04	—	—	211.2	NR	—

¹At 20 deg C organic + O₂ to CO₂(g) + H₂O (l)

²At normal boiling point.

Table 2. Heat Capacity Data

$$CP = A + B \times T \times 10^{-3} + C \times T^2 \times 10^{-7}$$

Where CP is cal/g/deg C and T is deg C

Component	Liquid			Vapor		
	A	B	C	A	B	C
C ₃ H ₆	—	—	—	0.339	1.007	-5.80
CO ₂	—	—	—	0.196	0.230	-1.59
AA	0.4833	0.418	34.67	0.428	5.106	-280.26
HAC	0.4790	0.524	11.28	0.703	-1.086	-8.34
O ₂	—	—	—	0.223	0.043	-0.06
N ₂	—	—	—	0.247	0.048	-0.08
H ₂ O	—	—	—	0.445	0.026	7.74
CH ₄	0.9985	0.057	16.52	0.512	0.816	0.55

4. Assume isothermal conditions.
5. Calculate the number of stages required, the height of this section, and the diameter.

5. Inclinerator

The composition and quantity of the absorber offgas will be based on the design and operation of the Oxidation reactor and the absorber. It is anticipated that the offgas will contain propylene, CO₂, acrylic acid, acetic acid, oxygen, nitrogen, and water. For environmental concerns, the offgas must be heated to destroy the hydrocarbons. To determine the operating parameters for the inclinerator, use the following assumptions:

1. CH₄ is available for heating.
2. 100% destruction of hydrocarbons to CO₂ and water.
3. Inclinerator firebox temperature is 700 deg C.
4. The stack gas is cooled to no lower than 10 deg C above its dew point to prevent dewpoint corrosion.
5. Steam is generated in a waste heat boiler (WHB) at 3,500kPa and 260 deg C.
6. 25% excess oxygen is supplied for combustion and safety.
7. Air is the source of oxygen and is supplied with an electrically driven fan. Assume a fan differential pressure of 7.5kPa.
8. Air is 21% oxygen and 79% nitrogen and the water content is 80% relative humidity. The temperature is 20 deg C.

6. Extraction/Solvent Recovery

The aqueous acid solution from the absorber bottoms is sent to the Separations section where it is contacted with an equal amount of solvent for countercurrent extraction of the acids in a centrifugal contactor. The extract is fed to a distillation column for stripping of the solvent and the remaining water. The distillate from this extract stripper is separated into an organic solvent layer and an aqueous layer in the reflux holding vessel. Part of the solvent layer is used for reflux, while the remainder is recycled to the extractors. The water layer is combined with the raffinate and sent to a raffinate stripper for further recovery of solvent.

There are two choices for the solvent. Solvent B requires less stages for extraction but has higher steam and process equipment costs to strip the solvent and water from the extract. Solvent A has lower steam and equipment costs for the stripping but requires more stages for extraction.

Use the equilibrium data supplied to determine the number of stages required to perform the extraction. The acids are to be treated as a single component and the recovery must be 97.5%.

Because of the difficulties involved with sizing multicomponent distillation columns, the extract stripper column is to be sized using data obtained through laboratory distillation experiments. Assume 100% recovery of acids to the extract stripper bottoms and negligible amounts of water and solvent in this stream.

The raffinate stripper column size and reboiler and condenser duties for each solvent case have also been supplied.

Determine which solvent should be used based on a net present value calculation.

7. Acrylic Acid Recovery

The separation of acrylic acid and acetic acid is done using normal distillation equipment. Because of the tend-

ency of acrylic acid to polymerize, it is necessary to maintain the temperature of the material below 90 deg C at all times. This is significant in the design of the distillation columns. In developing the column system for producing product acrylic acid and by-product acetic acid, the following assumptions should be made:

1. If more than one column is required, the streams to a column must be combined in such a way that the only inputs are one feed and the reflux stream, i.e., do not have two feeds to a single column.
2. Typical operating pressures at the top of a column are less than 200 mmHg.
3. The VLE data supplied is satisfactory for the temperatures and pressures in the process.

Determine the optimum design, recognizing the trade-offs between capital costs and operating expenses.

8. Equipment Pressure Drop Data

1. Condensers- vapor 1.3 kPa
2. Heat Exchangers- shell/tube- liquid 75 kPa
3. Oxidation Reactor- vapor 150 kPa
4. Piping negligible

9. Heat Transfer Coefficients

The following overall heat transfer coefficients may be assumed, kcal/hr/sq.m/deg C.

System	Overall Coefficient
Gas/Gas	50
Gas/Liquid	100
Gas/Boiling Liquid	200
Gas/Condensing Vapor	200
Liquid/Liquid	500
Liquid/Boiling Liquid	700
Liquid/Condensing Vapor	700
Boiling Liquid/Condensing Vapor	1000

ECONOMIC DATA

The economic data given here are adequate for the preliminary economic evaluations and should be used in preference to information from other sources. All costs are typical of the Gulf coast area.

All costs are in 1986 dollars. All evaluations should be done in terms of constant dollars, that is, ignore inflation.

Capital Costs

The total fixed capital investment can be estimated by multiplying the sum of the purchased equipment costs by a Lang factor of 5. Only the major pieces of equipment require design and costing. Purchased equipment costs for miscellaneous equipment which includes surge tanks, vacuum system, pumps, etc., can be estimated by the miscellaneous equipment cost located in the table.

Purchased Equipment Costs		
Equipment Item	Description	Cost (\$)
Absorber (Sec 2) Distillation Col.	304 SS Shell 316 SS sieve trays	$2900D(D+N)+(3.3D)^{1.19}N80$ $+(3.3D)^{0.54}1380+5700N$
Absorber (Sec 1)	Packed bed column	$D^2(3000+3400H)+D(9800+1500H)+14000$ $+350(3.3)^{1.19}+1400(3.3D)^{1.2}$
Air compressor	Centrifugal, electric drive	$EXP(.73Ln(P)-2.9)$
Combustion Air Fan	Centrifugal, electric drive	$EXP(0.556Ln(V)+6.988)$
Extraction	1600RPM, 316SS Centrifugal Contactor	120,000 (Number of theoretical stages)
Heat Exchangers	Carbon Steel Shell 304SS Tubes	$EXP(8.596+0.153Ln(A)+0.06(Ln(A))^3)$
Inclinerator	Thermal	$EXP(0.2Ln(G)+10.6)$
Oxidation Reactor	Carbon Steel Includes Catalyst	36000 (Number of tubes) ^{0.5}
Waste Heat Boiler	Carbon Steel Use for all steam gen.	$EXP(0.79Ln(S)+4.47)$
Waste Gas/ Boiler feed water heat exchanger (Economizer)	Carbon Steel Tubes Carbon Steel Shell	$EXP(8.698-0.0354Ln(A)+0.0689(Ln(A))$
Misc. Equipment	Surge Tanks, pumps, vacuum systems, etc.	0.1 (Purchase cost of major equipment items)

Where:

A = area in square meters

D = column diameter in meters

G = total inlet gas flowrate in actual cubic meters/hour

H = height of column in meters

N = number of trays

P = rated motor power in joules per hour

S = steam production rate in kilograms/hour

V = volume in cubic meters per minute at the inlet conditions

NOTE: $EXP(1) = e = 2.71828...$