**CHE654 – Plant Design Project #4**
**Semester 1, 2021**

# DESIGN OF AN ACETONE PRODUCTION PROCESS

(Courtesy of the Department of Chemical Engineering at West Virginia University)

## Introduction

Acetone is typically produced in commercial quantities as a by-product during the formation of phenol. However, acetone manufactured thus generally contains small amounts of the reactant benzene and the desired product phenol. In the past, these impurities were deemed to be within allowable limits. However, recent downward revisions of these limits by the US Food and Drug Administration has made alternative processes (which do not involve benzene) more attractive. We wish to begin the design of one such alternative process to produce 15,000 metric tons of acetone per year, using isopropyl alcohol as the reactant. Your job for this semester is to analyze a simplified acetone production process, to suggest profitable operating conditions, and to write a final report summarizing your findings. Note that optimization is NOT required in this design project.

## Process Description

Figure 1 is a preliminary process flow diagram (PFD) for the acetone production process. The raw material is isopropanol. The isopropanol (IPA) feed is a near azeotropic mixture with water at 88 wt % IPA at 25°C and 1 atm. The feed is heated, vaporized, and superheated in a heat exchanger (E-401), and it is then sent to the reactor (R-401) in which acetone is formed. The reaction that occurs is shown below. The reactor effluent is cooled and partially condensed in a heat exchanger (E-402), and it is then sent to a separation unit (V-401) in which all of the light gas (hydrogen) enters Stream 7 while the remaining components (acetone, IPA, and water) distribute. Some of the acetone in Stream 7 is recovered by absorbing it into pure water in T-401. The liquid in Stream 12 is distilled to produce "pure acetone" in Stream 13 and waste water (containing IPA) in Stream 14. The desired acetone production rate is 50,000 metric tons/year.

## Process Details

### Feed Streams

Stream 1: isopropyl alcohol, liquid, 88 wt % IPA, 12 wt % water, 1 atm, 25°C

Stream 9: distilled process water, 3 bar, 25°C

### Effluent Streams

Stream 11: off-gas stream to incinerator, credit may be taken for LHV of fuel

Stream 13: acetone product, liquid, 99.9 mol% purity, must contain 99.5 mol% of acetone in Stream 12

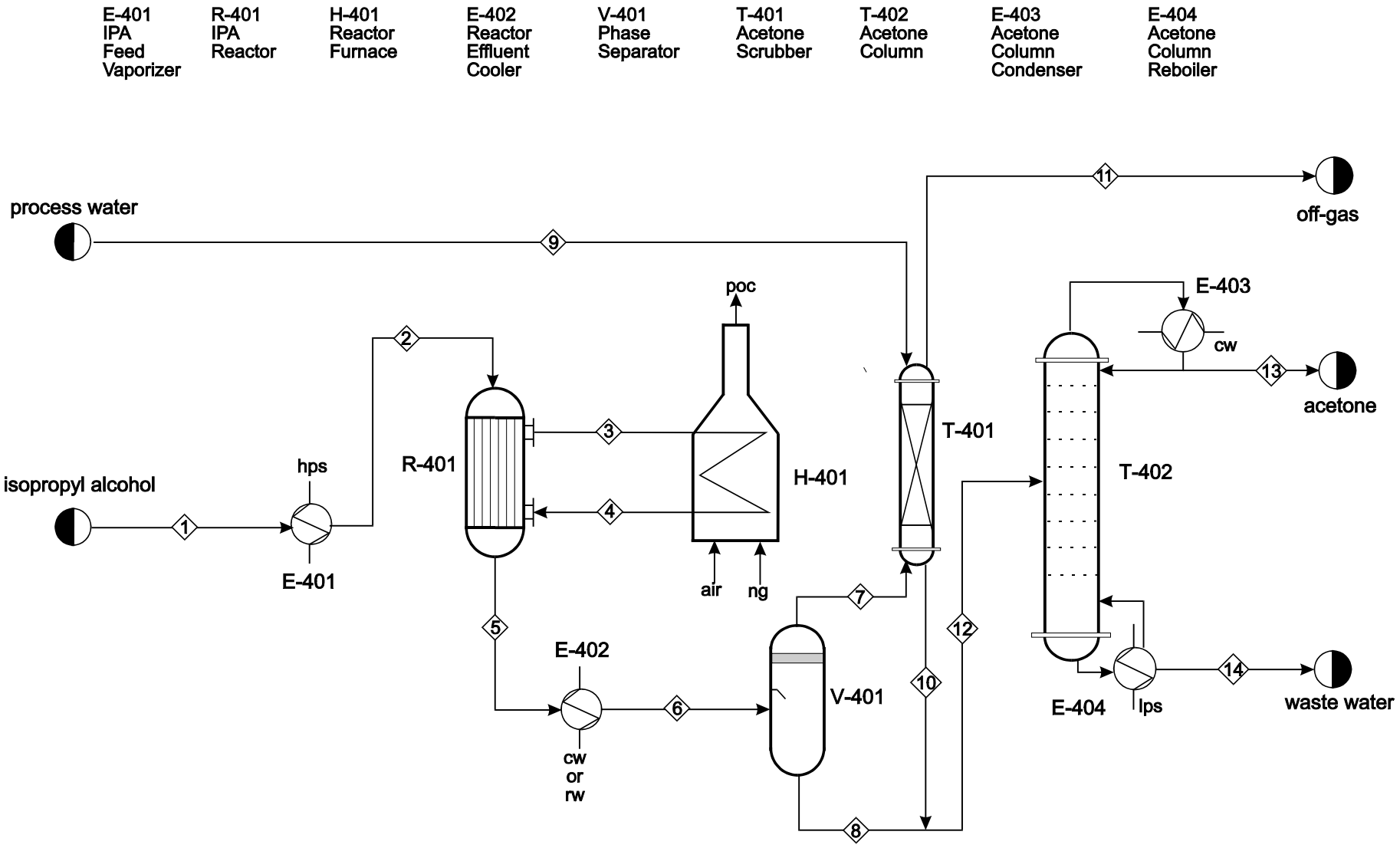



Figure 1: Process Flow Diagram for Acetone Production from Isopropyl Alcohol (Unit 400)

Stream 14: waste water stream, treatment cost \$50.00/$10^6$ kg
must contain less than 0.04 mole fraction IPA and acetone

**Equipment**

*Heat Exchanger (E-401):*

This unit heats, vaporizes, and superheats the feed to 235°C at 2.2 bar. A pump, which is not shown, increases the pressure of the feed to the indicated pressure.

*Reactor (R-401):*

Following development of a new catalyst, only the following reaction occurs:

$$\underset{\text{IPA}}{CH_3CHOHCH_3} \rightarrow \underset{\text{acetone}}{CH_3COCH_3} + H_2 \qquad (1)$$

The reaction occurs at 350°C, and the conversion at this temperature is 90% (if using a simple reactor model). The reactor exit pressure is 1.9 bar. The reaction is endothermic with heat being supplied by hot molten salt.

*Fired Heater (H-401):*

This unit heats the molten salt that provides heat to the reactor. Energy is supplied by combustion of natural gas, which may be assumed to be pure methane. The molten salt enters the fired heater at 360°C (Stream 3) and leaves the fired heater at 410°C (Stream 4). The heat capacity of molten salt is 1.56 J/g K.

*Heat Exchanger (E-402):*

This unit cools and partially condenses the reactor effluent. None of the hydrogen condenses. The exit pressure may be at any pressure below 1.6 bar and any temperature below 50°C that can be achieved by using cooling water (cw) or refrigerated water (rw) is possible.

*Separation Vessel (V-401):*

This unit disengages the vapor and liquid effluent from E-402. In this separator, all hydrogen in the feed enters the vapor phase, Stream 7. All other components distribute according to the appropriate property model you choose at the temperature and pressure of E-402. The combination of E-402 and V-401 is often called a flash operation.

*Absorber (T-401):*

Here, additional acetone is recovered by absorption into pure process water. The absorber operates at the same temperature and pressure as V-401. Stream 11 contains all of the hydrogen and the acetone and water which are not in Stream 10. Stream 10

contains all of the IPA in Stream 7, 95% of the water in Streams 7 and 9. The amount of acetone in Stream 10 can be calculated from:

$$\frac{y_{stream\,11}}{y_{stream\,7}} = \frac{1-A}{1-A^6} \tag{2}$$

where $y$ is the mole fraction of acetone,

$$A = \frac{L}{mV} \tag{3}$$

$L$ is the total molar flowrate of liquid in Stream 9, and $V$ is the total molar flowrate of liquid in Stream 7. The parameter $m$ is an equilibrium constant that is a function of temperature and pressure

$$m = \frac{\exp\left(10.92 - \frac{3598}{T}\right)}{P} \tag{4}$$

where $T$ is in Kelvin and $P$ is in atm.

*Distillation Column (T-402):*

In this distillation column, the acetone, IPA, and water in Stream 12 are separated. The column operates at 1.4 bar. Specifications are as follows. The acetone must be 99.9 mol% pure and 99.5 mol% of the acetone in the feed must be recovered in Stream 13. Stream 14 contains most of the water and IPA from Stream 12.

*Heat Exchanger (E-403):*

In this heat exchanger, the contents of Stream 13 are condensed from saturated vapor to saturated liquid at a rate three times the flow of Stream 13. The cost is for the amount of cooling water needed to remove the necessary energy.

*Heat Exchanger (E-404):*

In this heat exchanger, you may assume that one-half of the flow of Stream 14 is vaporized from saturated liquid to saturated vapor at 1.4 bar and is returned to the column. The cost is for the amount of low-pressure steam needed to supply the necessary heat.

*An additional distillation column (T-403):*

To make your process more economically attractive, adding an additional distillation column to process Stream 14 further is highly suggested. This additional column can recover a near azeotropic mixture of water and IPA (88 wt% IPA – with all of the acetone remaining in Stream 14) out of the top, with residual water and IPA out the bottom. The IPA/water top product is sent to combine with the fresh feed at the beginning of the process

while the bottom product goes to waste water treatment. This distillation column operates at 1.2 bar and needs two heat exchangers with similar energy specifications to E-403 and E-404.

*Other Equipment:*

It is required for two streams that mix to be at identical pressures. Pressure reduction may be accomplished by adding a valve. These valves are not shown on the attached flowsheet, and it may be assumed that additional valves can be added as needed at no cost. Flow occurs from higher pressure to lower pressure. Pumps increase the pressure of liquid streams, and compressors increase the pressure of gas streams. You may assume that a pump exists wherever you need one.

**Design of Heat Exchangers, E-401 and E-402**

A detailed design of E-401 and E-402 is required for base-case conditions. It should be assumed that cooling water is available at the conditions specified in the Appendix of this problem statement. For this heat exchanger design, the following information should be provided:

- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Diameter, tube-wall thickness, shell-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the two exchangers should be included along with a set of comprehensive calculations in an appendix for the design of the heat exchangers. You should use ASPEN Exchanger Design & Rating (EDR) in the ASPEN Plus simulator to carry out the detailed design.

## Economic Analysis

When evaluating alternative cases, you should carry out an economic evaluation and profitability analysis based on a number of economic criteria such as payback period, internal rate of return, and cash flow analysis. In addition, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

$$\text{EAOC} = -(\text{product value} - \text{feed cost} - \text{other operating costs} - \text{capital cost annuity})$$

A negative EAOC means there is a profit. It is desirable to minimize the EAOC; i.e., a large negative EAOC is very desirable, although you are not being asked to carry out optimization.

The cost for acetone is \$0.88/kg. The cost for IPA is \$0.72/kg IPA in the feed solution. The value for hydrogen is \$35/1000 std $m^3$.

Other operating costs are utilities, such as steam, cooling water, natural gas, and electricity.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed cost of plant construction. The capital cost annuity is defined as follows:

$$capital\ cost\ annuity = FCI\frac{i(1+i)^n}{(1+i)^n - 1}$$

where *FCI* is the installed cost of all equipment; $i$ is the interest rate, $i = 0.15$; and $n$ is the plant life for accounting purposes, $n = 10$.

For detailed sizing, costing, and economic evaluation including profitability analysis, you may use the Aspen Process Economic Analyzer (formerly Aspen Icarus Process Evaluator) in Aspen Plus Version 7. However, it is also a good idea to independently verify the final numbers based on other sources such as cost data given below.

## Other Information

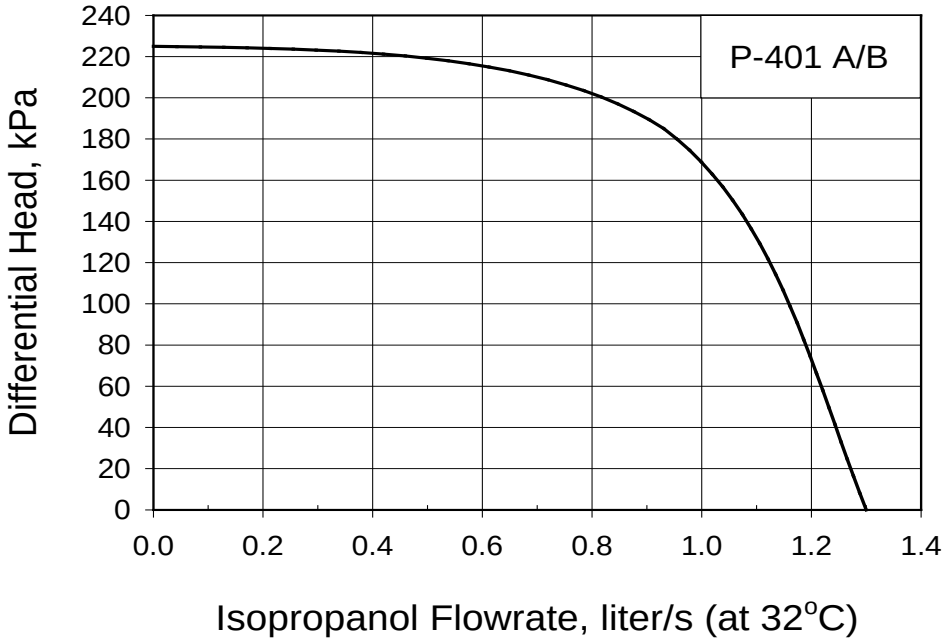
You should assume that a year equals 8,000 hours. This is about 330 days, which allows for periodic shut-down and maintenance.

## Final Comments

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. You may need to fill in some missing data by doing a literature search, Internets search, or making assumptions. The possibility exists that as you work on this problem, your questions will require revisions and/or clarifications of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.

Moreover, in some areas (e.g. sizing/costing) you are given more data and information than what is needed. You must exercise engineering judgment and decide what data to use. Also you should also seek additional data from the literature or Internet to verify some of the data, e.g. the prices of products and raw materials.

## Additional Data



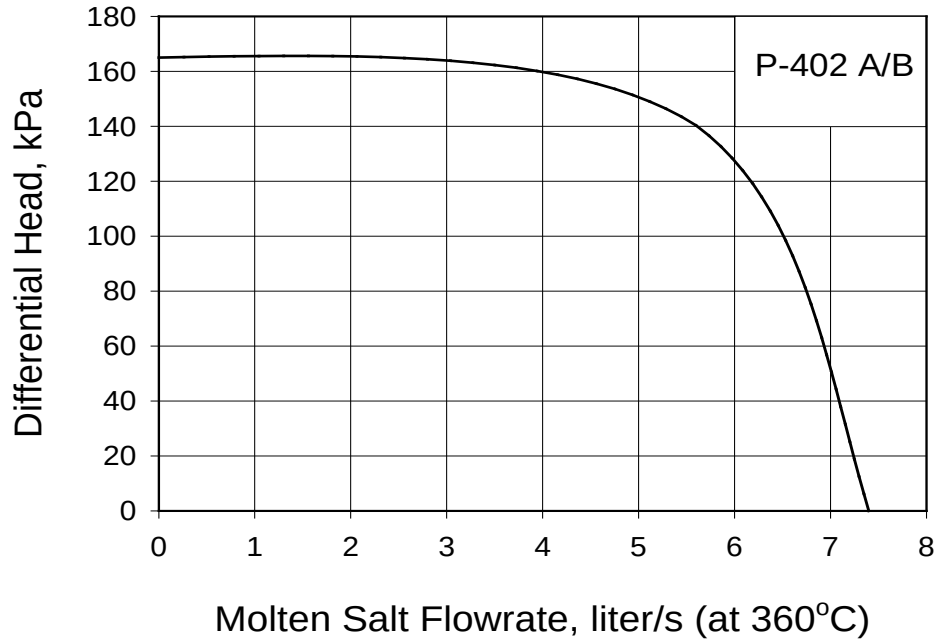




Figure 2: Pump Curves for P-401 A/B and P-402 A/B

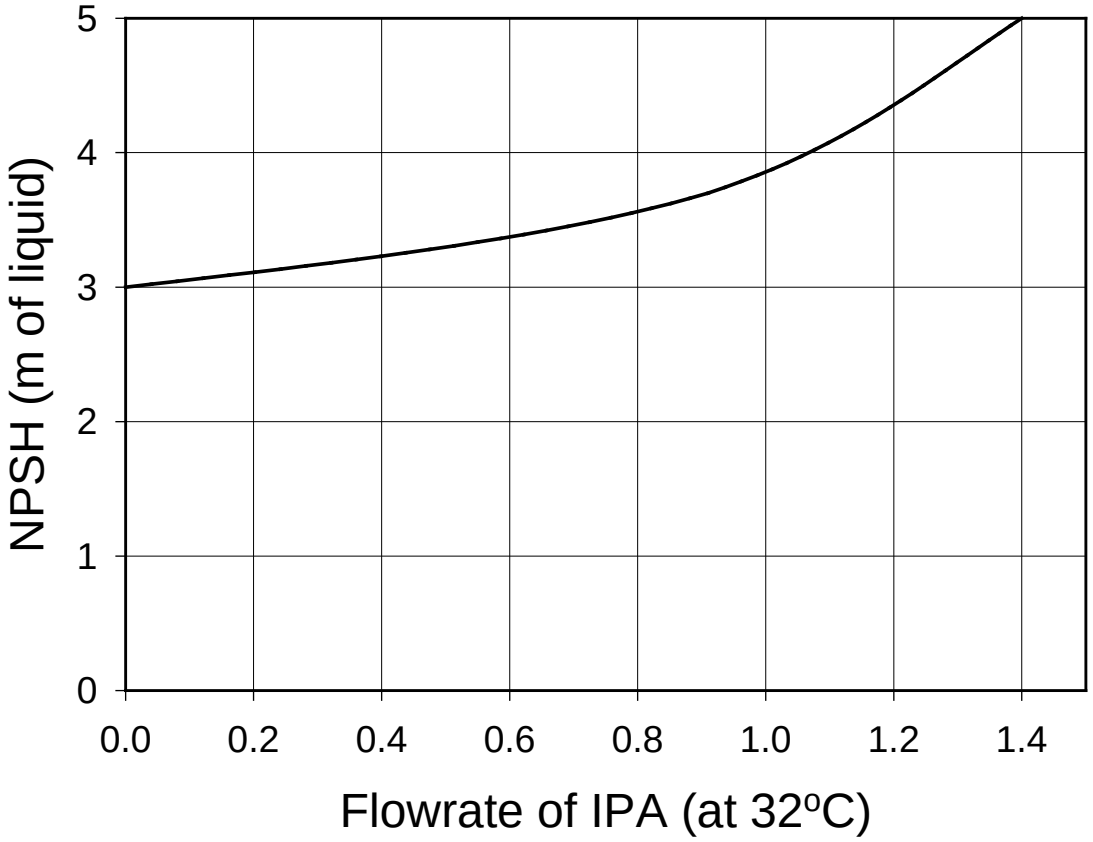



Figure 3: NPSH required by Pump, P-401 A/B, IPA Feed Pump

## Reaction Kinetics

The main reaction for producing acetone is

$$\underset{\text{isopropanol}}{(CH_3)_2CHOH} \rightarrow \underset{\text{acetone}}{(CH_3)_2CHO} + H_2$$

and the kinetics for this reaction are given below:

$$-r_{IPA} = k_1 C_{IPA} \qquad \frac{\text{mol IPA}}{\text{m}^3\text{catalyst}\cdot\text{s}}$$

where

$$k_1 = 1.76\times10^5 \exp\left[-\frac{60{,}000}{RT}\right] \qquad \frac{\text{m}^3\text{gas}}{\text{m}^3\text{catalyst}\cdot\text{s}}$$

$$C_{IPA} = \frac{\text{mol IPA}}{\text{m}^3\text{gas}}$$

These kinetics are only valid if the actual conversion does not exceed 85% of the equilibrium conversion at reactor conditions. Although, several side reactions are possible, none of them take place to any considerable extent. The activation energy in the kinetic expression above is in units of kJ/kmol.

## Catalyst Information

Catalyst physical properties are given below:

density of the inert catalyst, $\rho_{ci}$ = 2500 kg/m$^3$
density of solid catalyst, $\rho_c$ = 2500 kg/m$^3$
packed bed voidage of the cylindrical pellets = 0.5
void fraction of the spherical particles at minimum fluidizing conditions = 0.55
particle diameter, $d_p$ = 100 μm

## Heat Exchangers

For heat exchangers, use the following approximations for heat transfer coefficients to allow you to determine the heat transfer area:

| situation | $h$ (W/m$^2$°C) |
|---|---|
| condensing steam | 6000 |
| condensing organic | 1000 |
| boiling water | 7500 |
| boiling organic | 1000 |
| flowing liquid | 600 |
| flowing gas | 60 |

## Cost Data

## Utility Costs

| | |
|---|---|
| Low Pressure Steam (618 kPa saturated) | $6.62/1000 kg |
| Medium Pressure Steam (1135 kPa saturated) | $7.31/1000 kg |
| High Pressure Steam (4237 kPa saturated) | $8.65/1000 kg |
| Natural Gas (446 kPa, 25°C) | $3.00/GJ |
| Fuel Gas<br>use this price for fuel gas credit | $2.75/GJ |
| Electricity | $0.06/kW h |
| Boiler Feed Water (at 549 kPa, 90°C) | $2.54/1000 kg |
| Cooling Water<br>available at 516 kPa and 30°C<br>return pressure ≥ 308 kPa<br>return temperature is no more than 15°C above the inlet temperature | $0.16/GJ |
| Refrigerated Water | $1.60/GJ |

available at 516 kPa and 10°C
return pressure ≥ 308 kPa
return temperature is no higher than 20°C

| | |
|---|---|
| Deionized Water<br>available at 5 bar and 30°C | $1.00/1000 kg |
| Waste Treatment of Off-Gas | incinerated - take fuel credit |
| Refrigeration | $60/GJ |

## Equipment Costs (Purchased)

| | |
|---|---|
| Pumps | $630 (power, kW)$^{0.4}$ |
| Heat Exchangers | $1030 (area, m$^2$)$^{0.6}$ |
| Compressors | $770 (power, kW)$^{0.96}$ + 400 (power, kW)$^{0.6}$ |
| Turbine | $2.18×10$^5$ (power output, MW)$^{0.6}$<br>assume 65% efficiency |
| Fired Heater | $635 (duty, kW)$^{0.8}$<br>assume 80% thermal efficiency<br>assume can be designed to use any organic compound as a fuel |
| Vessels | $[1.67(0.959 + 0.041$*P* - 8.3×10$^{-6}$*P*$^2$)]×10$^z$<br>$z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$<br>*D* = diameter, m  0.3 m < *D* < 4.0 m<br>*L* = height, m  *L*/*D* < 20<br>*P* = absolute pressure, bar |
| Catalyst | $2.25/kg |
| Reactor | packed bed: $3,000/m$^2$ of heat transfer surface<br>fluidized bed: $10,000/m$^2$ of heat transfer surface |
| Packed Tower | Cost as vessel plus cost of packing |
| Packing | $(-110 + 675$*D* + 338*D*$^2$)*H*$^{0.97}$<br>*D* = vessel diameter, m; *H* = vessel height, m |
| Tray Tower | Cost as vessel plus cost of trays |
| Trays | $(187 + 20$*D* + 61.5*D*$^2$)<br>*D* = vessel diameter, m |
| Storage Tank | $1000*V*$^{0.6}$ |

$V$ = volume, $m^3$

It may be assumed that pipes and valves are included in the equipment cost factors. Location of key valves should be specified on the PFD.

## Equipment Cost Factors

| | | |
|---|---|---|
| Pressure (absolute) | < 10 atm, 0.0<br>10 - 20 atm, 0.6<br>20 - 40 atm, 3.0<br>40 - 50 atm, 5.0<br>50 - 100 atm, 10 | does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects |
| Carbon Steel | 0.0 | |
| Stainless Steel | 4.0 | |

Total Installed Cost = Purchased Cost (4 + material factor + pressure factor)

## References


1. Turton, R., R.C. Bailie, W. B. Whiting and J. A. Shaeiwitz, *Analysis, Synthesis and Design of Chemical Processes*, Prentice-Hall, Upper Saddle River, NJ,1998.

2. Felder, R. M. and R. W. Rousseau, *Elementary Principles of Chemical Processes*, 2nd edition, Wiley, New York, 1986.

3. Reid, R. C., J. M. Prausnitz and B. E. Poling, *The Properties of Gases and Liquids*, 4th edition, McGraw Hill, New York, 1987.

4. Perry, R. H. and D. Green, eds., *Perry's Chemical Engineers' Handbook*, 7th edition, McGraw-Hill, New York, 1997.