# Energy Balances, Numerical Methods
# Design Project

# Production of Acetone

## 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 according to Raoult's Law. 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 15,000 metric tons/yr.

## 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

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

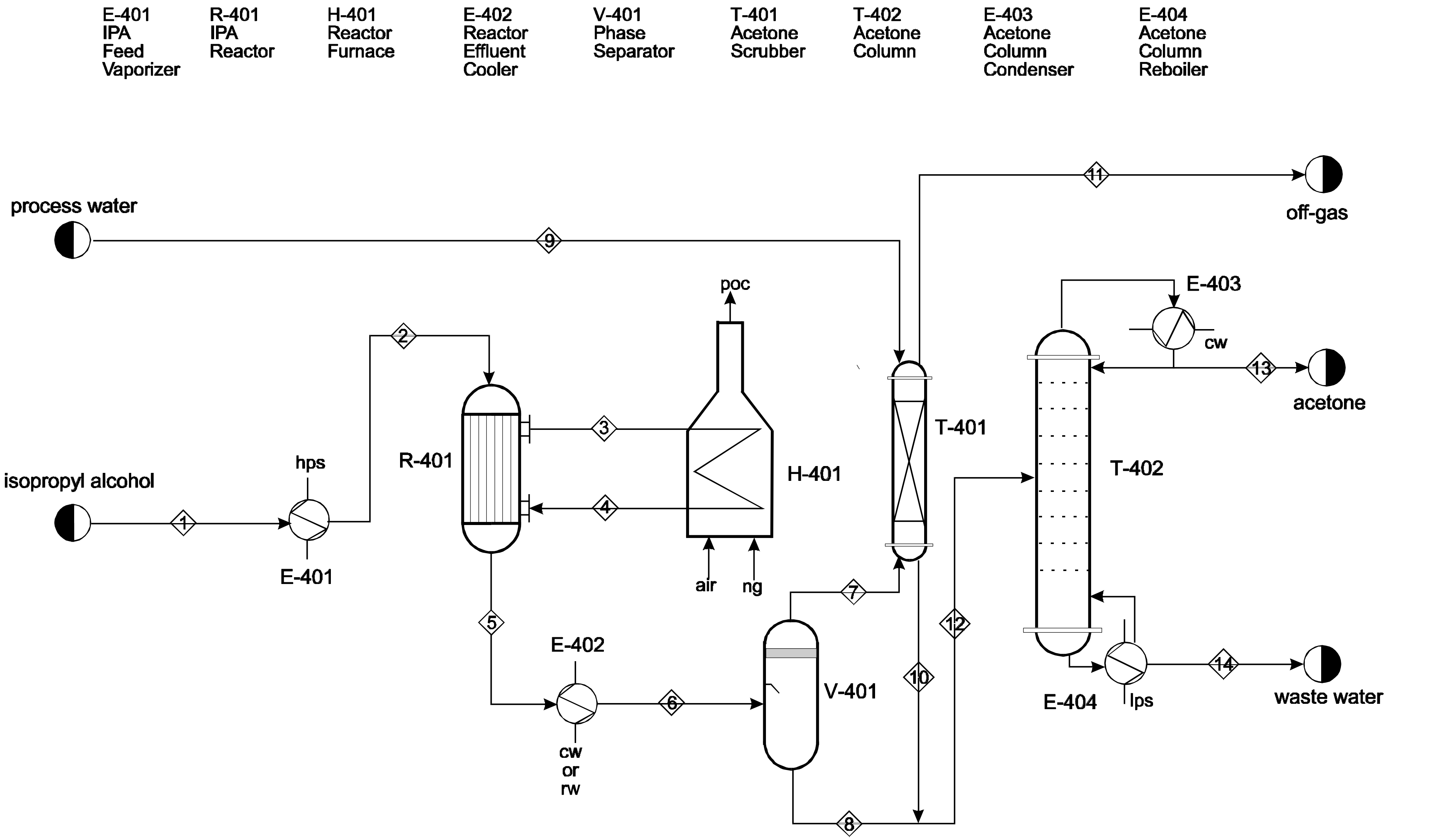


Figure 1: Process Flow Diagram for Acetone Production from Isopropyl Alcohol (Unit 400)

**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 and which you do not have to be concerned with this semester, increases the pressure of the feed to the indicated pressure.

Reactor (R-401):

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

$$\underset{\text{IPA}}{CH_3CHOHCH_3} \rightarrow \underset{\text{acetone}}{CH_3COCH_3} + H_2 \tag{1}$$

The reaction occurs at 350°C, and the conversion at this temperature is 90%. 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 Raoult's Law 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:

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

where $y$ is the mole fraction of acetone,

$$A = \frac{L}{mV} \qquad (3)$$

$L$ 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

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

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):

You may choose to add an additional distillation column to process Stream 14 further. This 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. If you choose to do this, you must recycle the IPA/water top product to the beginning of the process. The bottom product goes to waste water treatment. This distillation column needs two heat exchangers with similar energy specifications to E-403 and E-404. This distillation column operates at 1.2 bar. You should only include this column if you decide it to be economically attractive

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 where ever you need one. For this semester only, there is no cost for pumps.

## Equipment Costs

The equipment costs for the acetone plant are given below. Each cost is for an individual piece of equipment, including installation.

| **Equipment** | **Installed Cost in millions of $** |
|---|---|
| Reactor, R-401 | 1.5 |
| Absorber, T-401 | 0.03 |
| Acetone distillation column T-402 including reboiler and condenser | 2.8 |
| IPA distillation column T-403 (if added) including reboiler and condenser | 0.1 |
| Vessel, V-401 | 0.07 |
| Any heat exchanger | 0.05 |

Fired heater installed cost in dollars:

$$11 \times 10^{x}$$

where

$$x = 2.5 + 0.8 \log_{10} Q$$

where $Q$ is the heat duty in kW

## Utility Costs

| | |
|---|---|
| Low-Pressure Steam (446 kPa, saturated) | \$5.00/1000 kg |
| Medium-Pressure Steam (1135 kPa, saturated) | \$7.31/1000 kg |
| High-Pressure Steam (4237 kPa, saturated) | \$8.65/1000 kg |
| Natural Gas or Fuel Gas (446 kPa, 25°C) | \$3.00/GJ |
| Electricity | \$0.05/kW h |
| Boiler Feed Water (at 549 kPa, 90°C) | \$2.54/1000 kg |
| Cooling Water | \$0.16/GJ |

Cooling Water: available at 516 kPa and 30°C
return pressure ≥ 308 kPa
return temperature should be no more than 15°C above the inlet temperature

Refrigerated Water — \$1.60/GJ
available at 516 kPa and 10°C
return pressure ≥ 308 kPa
return temperature is no higher than 20°C

Process Water — \$0.04/1000 kg
available at 300 kPa and 25°C

## Data

Use data from Reference [1] or from any handbook (such as Reference [2]). The following data are not readily available in these references.

Liquid Heat Capacity
For IPA: 145 J/mole K

Vapor Heat Capacity
for IPA: $27.87 + 0.176 + 2.12\times 10^{-4}T^{2} - 4.09\times 10^{-7}T^{3}$ J/mole K $T$ (K)

Vapor Pressures – Antoine's Equation constants

$$\ln\ p^{*} = A - \frac{B}{T + C} \qquad (5)$$

($p^{*}$ in mm Hg, $T$ in K)

| | ***A*** | ***B*** | ***C*** |
|---|---|---|---|
| IPA | 17.664 | 3109.3 | -73.546 |
| acetone | 16.732 | 2975.9 | -34.523 |

Normal heat of vaporization
for IPA: 56,900 kJ/kmole

## Economic Analysis

When evaluating alternative cases, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

EAOC = -(product value - feed cost - other operating costs - 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.

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. A list of capital costs for all pieces of equipment will be provided by early March.

The capital cost annuity is defined as follows:

$$\textit{capital cost annuity} = 0.2(\textit{capital cost})$$

## Optimization

We will learn optimization methods in numerical methods class. The objective function (EAOC) is defined above. It is your responsibility to define appropriate decision variables. If there are too many decision variables to do a reasonable optimization, it is your responsibility to determine, with appropriate justification, which ones most significantly affect the objective function and focus on only those decision variables.

## Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shut-down and maintenance.

## Deliverables

Each group must deliver a report written using a word processor. The report should be clear and concise. The format is explained in a separate document. Any report not containing a labeled PFD and a stream table will be considered unacceptable. The stream table must include temperature, pressure, phase, total mass flowrate, total molar flowrate, and component molar flowrates. When presenting results for different cases, graphs are generally superior to tables. The report appendix should contain details of calculations for the optimal case. These calculations may be (neatly) hand-written. Calculations that can not be followed easily will lose credit. Refer to the document entitled *Written Design Reports* for more information.

Each group will give an oral report in which the results of this project are presented in a concise manner. The oral report should be no more than 15 minutes, and each group member must speak. A 5-10 minute question-and-answer session will follow. Instructions for presentation of oral reports will be provided in a separate document entitled *Oral Reports*. However, the best way to learn how to present an oral report, other than actually presenting one, is to make time to see some of the oral reports presented by the juniors the week before you are to present your report. The presentations will most likely be on Wednesday, April 21, 1999, between 11:00 a.m. and 3:00 p.m.

As mentioned in the cover memo, the written project report is due on Monday, April 26, 1999, at 1:00 p.m. The oral reports will be Monday, April 26, 1999 (ChE 38 class) and Wednesday, April 28, 1999 (ChE 41 class). There will be a project review on Thursday, April 30, 1999 (ChE 38 class). In addition, everyone must attend the senior design presentation on Tuesday, April 27, 1999, unless you have organic chemistry or physics lab at that time. Furthermore, attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the lounge). Failure to attend any of the above required sessions will result in a decrease in one letter grade (per occurrence) from your project grade in both ChE 38 and ChE 41.

Anyone not participating in this project will automatically receive an F for ChE 38, regardless of other grades earned in this classes.

## Revisions

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. 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.

## References

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

2. Perry, R. H. and D. Green, eds., *Perry's Chemical Engineering Handbook (7th ed.)*, McGraw-Hill, New York, 1997.