# Energy Balances and Numerical Methods
# Design Project

## Production of Acrylic Acid

## Process Description

Figure 1 is a preliminary process flow diagram (PFD) for the acrylic acid production process. The raw materials are propylene and oxygen. Steam in added to provide thermal ballast. The propylene feed may be assumed pure vapor at 446 kPa. The air feed, which may be considered to contain only oxygen, nitrogen, and water is also at 446 kPa. The steam is saturated at 446 kPa. The feeds are mixed and sent to the reactor (R-301) in which acrylic acid is formed. There reactions which occur are shown below. The reactor effluent is sent to a separation unit (S-301) in which all light gases (oxygen, nitrogen, carbon dioxide, and propylene) are separated as vapor in Stream 7. Stream 7 is split into Streams 8 and 9. Stream 8 is a recycle stream containing propylene, oxygen, nitrogen, and carbon dioxide. A pump is required in this stream which is not shown. Stream 9 is incinerated. Stream 10, containing water and acrylic acid is sent to a distillation column (T-301) to produce purified acrylic acid. The desired acrylic acid production rate is 50,000 metric tons/yr.

## Process Details

### Feed Streams

Stream 1: propylene, pure vapor, 25°C and 446 kPa

Stream 2: air at 218°C and 446 kPa
(it has been compressed from atmospheric pressure causing the temperature increase - the annual cost for this compression is $1.22M per compressor)
water present in amount to saturate air at 25°C and 1 atm

Stream 3: low-pressure steam

Stream 4: feed mixture should have the following components:
air (containing oxygen, nitrogen, and water vapor) 55 mole %
steam (added as steam) 40 mole%
propylene 5 mole %
you must determine the stream temperature

### Effluent Streams

Stream 9: waste gas stream to incinerator, credit may be taken for LHV of fuel

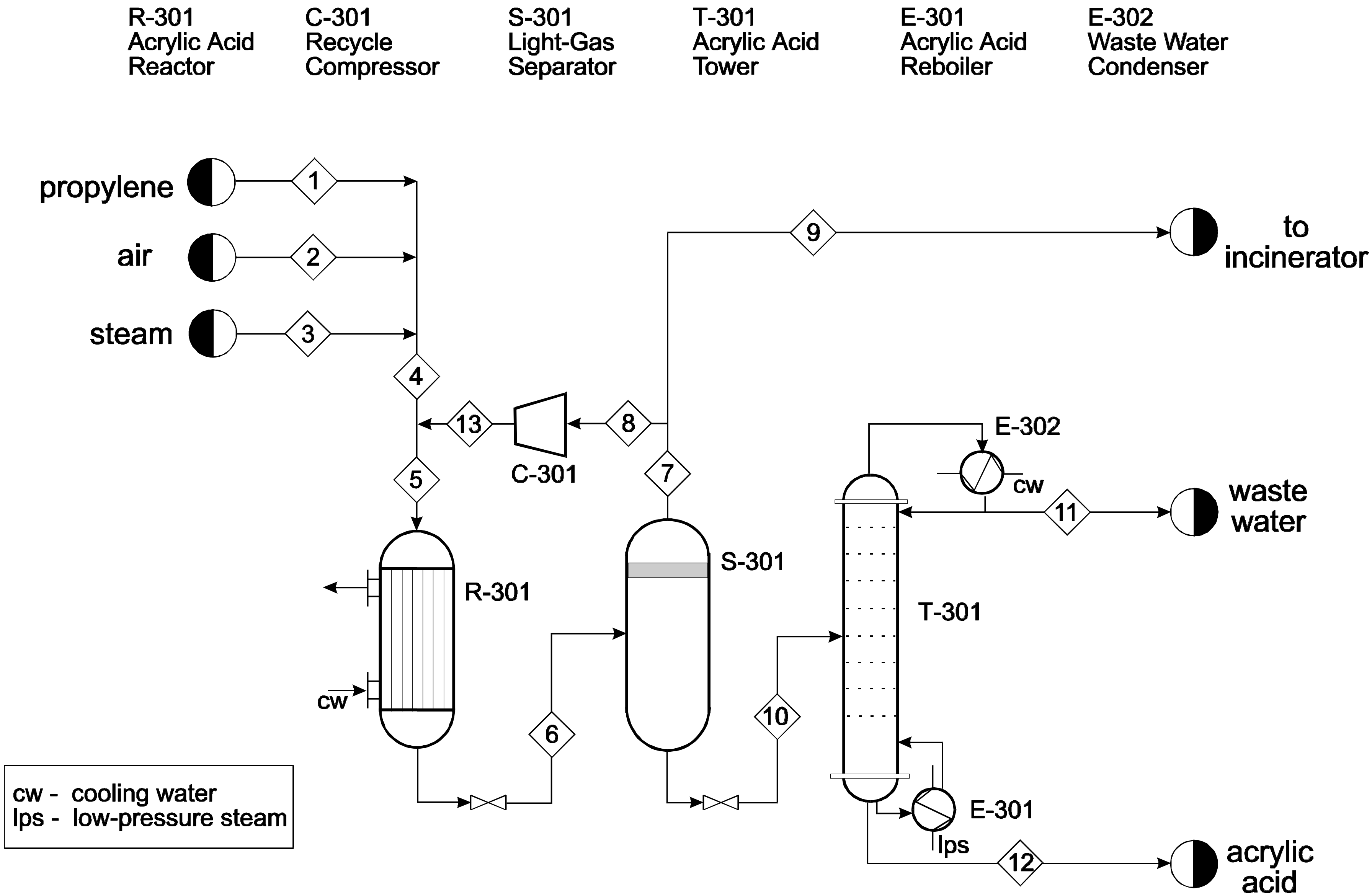


Figure 1: Process Flow Diagram for Acrylic Acid Production

Stream 11: waste water stream, treatment cost $50.00/10^6 kg
must contain less than 0.05 wt % acrylic acid

Stream 12: acrylic acid product, 99.9 wt% purity.

**Equipment**

Reactor (R-301):

The following reactions occur:

$$C_3H_6 \quad + \quad 1.5O_2 \;\rightarrow\; C_3H_4O_2 + H_2O$$

propylene acrylic acid

$$C_3H_6 \quad + \quad 4.5O_2 \;\rightarrow\; 3CO_2 + 3H_2O$$

Selectivities and conversions at various temperatures are given in Table 1. These values are for the reactor operating pressure of 446 kPa and are independent of the amount of oxygen present, as long as propylene is the limiting reactant. Part of your assignment is to determine the best exit reactor temperature.

**Table 1**
**Selectivity and Conversion at Different Temperatures**

| Temperature (°C) | Selectivity (moles acrylic/ moles $CO_2$) | Conversion of Propylene |
|---|---|---|
| 200 | 10.0 | 0.04 |
| 250 | 10.0 | 0.05 |
| 300 | 9.77 | 0.11 |
| 350 | 8.91 | 0.22 |
| 400 | 7.24 | 0.36 |
| 450 | 4.90 | 0.50 |
| 500 | 2.45 | 0.63 |
| 550 | 0.891 | 0.76 |
| 600 | 0.655 | 0.83 |
| 650 | 0.610 | 0.86 |

Separator (S-301):

In this separator, all components other than acrylic acid and water exit in Stream 7. The acrylic acid and water vapor are partitioned between Streams 7 and 10 according to Raoult's law. Part of your task is to determine the optimum temperature and pressure for this separator. The separator pressure must be below 446 kPa. Note: The vapor pressure expression given in last semester's design project is not applicable here. You must determine such an expression on your own.

Distillation Column (T-301):

In this distillation column, the water and acrylic acid in Stream 10 are separated. The column operates at vacuum conditions. Specifications are as follows. The column pressure is determined by the boiling point of acrylic acid at its maximum allowable temperature, 90°C. This is also the temperature of Stream 12. The temperature of Stream 11 is the boiling point of water at the pressure of the column. Energy requirements are described with the heat exchange equipment, below.

Heat Exchanger (E-301):

In this heat exchanger, you may assume that one-half of the flow of Stream 12, containing pure acrylic acid, is vaporized from saturated liquid to saturated vapor at 90°C. The cost is for the amount of low-pressure steam needed to supply the necessary heat.

Heat Exchanger (E-302):

In this heat exchanger, water is condensed from saturated vapor to saturated liquid at a rate three times the flow of Stream 11. The cost is for the amount of refrigerated water needed to remove the necessary energy.

## Equipment Costs

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

| **Equipment** | **Installed Cost in millions of $** |
|---|---|
| reactor | 7.4 |
| compressor | 7.8 |
| distillation column (not including reboiler and condenser) | 0.4 |
| vessel | 0.2 |
| any heat exchanger | 0.1 |
| miscellaneous equipment not shown on the process flow diagram | 0.1 |

If you cool Stream 6 as part of the flash, you will need to add the cost of a heat exchanger to the cost of a vessel to calculate the installed cost of S-301.

## 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
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

## 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
Assume that the liquid heat capacity for benzene given in Reference [1] is valid for all other organic liquids.

Vapor Heat Capacity
for acrylic acid: $1.742 + 0.3191T - 2.352 \times 10^{-4}T^2 + 6.975 \times 10^{-8}T^3$ J/mole K $T$ (K)

Vapor Pressures
Vapor pressures may be interpolated or extrapolated from the following data:

| | normal boiling point | additional vapor pressure point | |
|---|---|---|---|
| | *T* (K) | *T* (K) | *P* (MPa) |
| propylene | 225 | 365 | 4.620 |
| acrylic acid | 391 | 615 | 5.674 |

Normal heat of vaporization
for acrylic acid: 32.94 kJ/mole

Heat of formation
for acrylic acid: -336,500 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 costs for acrylic acid (the product) and propylene (the feed) should be obtained from the *Chemical Marketing Reporter*, which is in the Evansdale Library.

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 Spring Break. You will learn to calculate the annuity value in ChE 38.

## Optimization

We will learn optimization methods in ChE 38. 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.

You should assume that two streams that mix must 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. In general, flow occurs from higher pressure to lower pressure. Pumps increase the pressure of liquid streams, and compressors increase the pressure of gas streams. The two locations where pumps are needed are Streams 11 and 12, to remove material from the tower operating at vacuum conditions. A small compressor or blower is also needed in Stream 8. For purposes of this design only, you may assume that Stream 8 is at whatever pressure is needed to allow it to mix with Stream 4, and that there is no cost associated with this pressure increase.

For this semester only, assume the following relationship for a compression or expansion operation:

$$\left(\frac{T_{out}}{T_{in}}\right)=\left(\frac{P_{out}}{P_{in}}\right)^{0.286}$$

## 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 which 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 22, 1998, between 11:00 am and 3:00 pm.

As mentioned in the cover memo, the written project report is due upon presentation of the oral report. The oral reports will be Monday, April 27, 1998 (ChE 38 class) and Wednesday, April 29, 1998 (ChE 41 class). There will be a project review on Friday, May 1, 1998 (ChE 41 class). In addition, everyone must attend at least one (and preferably both) of the senior design presentations, either on Tuesday, April 28, 1998, or on Thursday, April 30, 1998 (substitutes for Thursday ChE 38 class). 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 (6th ed.)*, McGraw-Hill, New York, 1984.