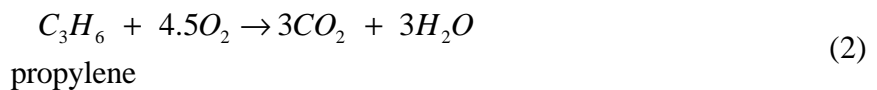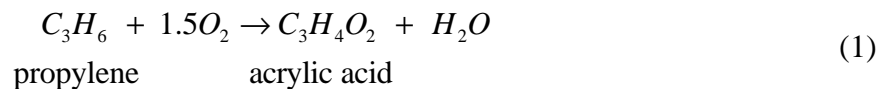# Material Balances
Design Problem -- Acrylic Acid Production

Acrylic acid is produced by the catalytic partial oxidation of propylene in the presence of steam at elevated temperature and ambient pressure. We wish to begin the design of a process to produce 50,000 metric tons of acrylic acid per year. Your job for this semester is to analyze a simplified acrylic acid production process and to suggest profitable operating conditions.

Figure 1 is a flow diagram of a simplified process for acrylic acid production. Figure 1 is also simplified; in particular, pumps (to raise the pressure) and other equipment extraneous to the present level of design are not included. In the simplified process, propylene, air (a source of oxygen), and steam are mixed and fed to the reactor at 4.3 atm. The reactions occurring within the reactor are as follows:

$$C_3H_6 + 1.5O_2 \rightarrow C_3H_4O_2 + H_2O$$
$$\text{propylene} \qquad \text{acrylic acid}$$

$$(1)$$

$$C_3H_6 + 4.5O_2 \rightarrow 3CO_2 + 3H_2O$$
$$\text{propylene}$$

$$(2)$$

Eq. (1) is the desired acrylic acid production reaction and Eq. (2) is the undesired propylene combustion reaction. The outlet stream from the reactor is then flashed to a lower pressure and a different temperature, such that some of the water and some of the acrylic acid form a liquid phase. The vapor phase and the liquid phase leave the light-gas separator in separate streams. The vapor phase is incinerated. The liquid phase is further separated into pure acrylic acid and pure (waste) water.

Process Streams

Stream 1: This stream may be assumed to be pure propylene (polymer grade).

Stream 2: This stream is compressed air containing water vapor at an amount that would saturate the air at 25⌒C and 1 atm. Air is assumed to consist of 21 mol% oxygen and 79 mol% nitrogen on a water-vapor-free basis.

Stream 3: This stream is steam at 160⌒C and 6 atm.

Stream 4: This is a mixture of Streams 1-3. It should contain the following mole fractions: propylene - 0.05, air (includes oxygen, nitrogen, and water vapor) - 0.55, steam added in Stream 3 - 0.40

Stream 5: This vapor stream is the reactor effluent. The valve in this stream lowers the pressure and changes the temperature for the separators.
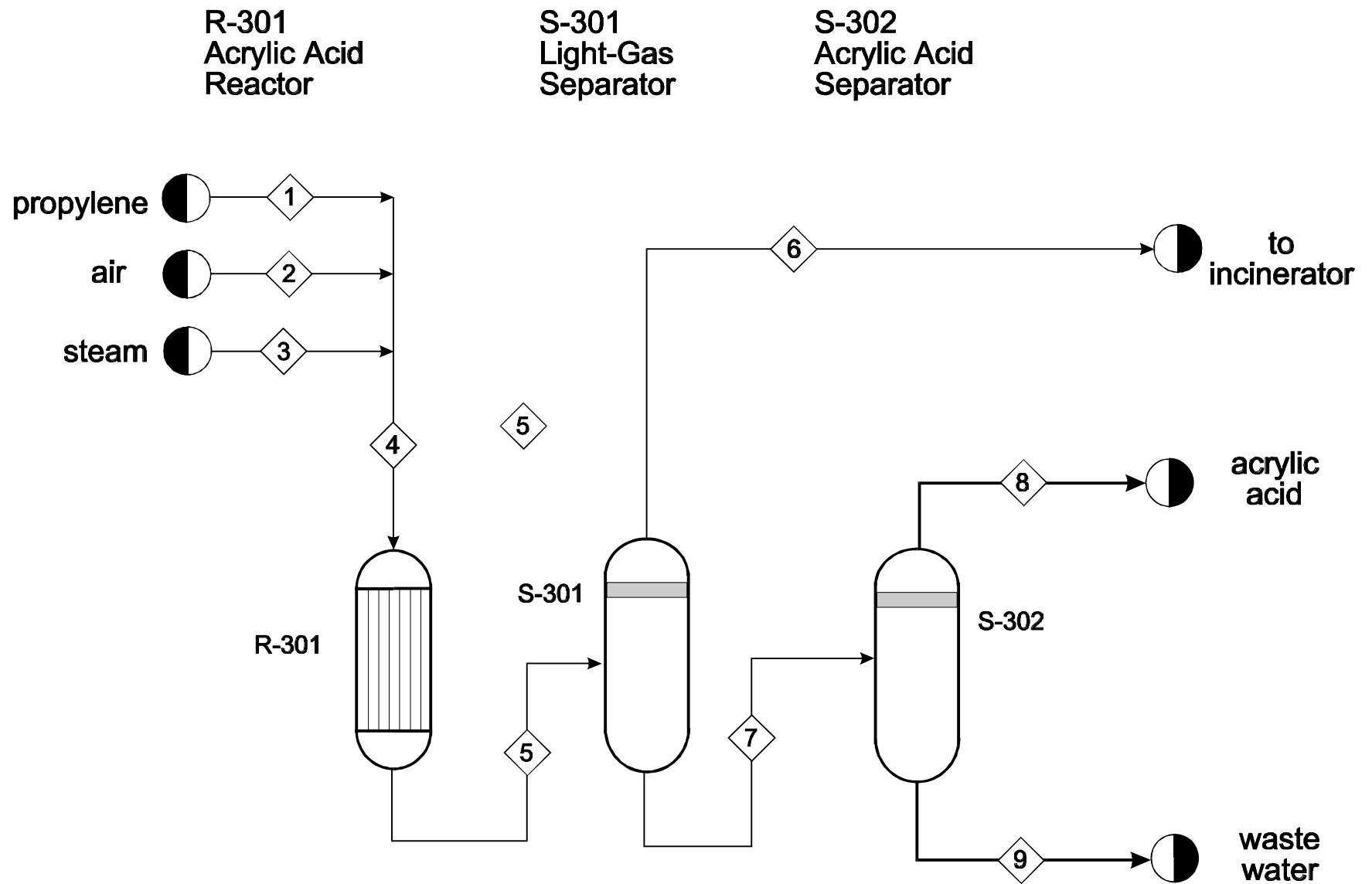
Figure 1: Process Flow Diagram for Acrylic Acid Production

Stream 6: This vapor stream contains all components in Stream 5 other than water and acrylic acid.
The water and acrylic acid are partitioned between Streams 6 and 7 according to Raoult's law.

Stream 7: This liquid stream contains only water and acrylic acid.

Stream 8: This vapor stream contains pure acrylic acid.

Stream 9: This liquid stream contains pure water.

Process Units

Acrylic Acid Reactor (R-301)

In this reactor, the reactions in Eqs. (1) and (2) occur. The selectivity and conversion at various temperatures are given in Table 1. These values are for the reactor operating pressure of 4.3 atm and are independent of the amount of oxygen present, as long as propylene is the limiting reactant.

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	0.85

Light-Gas Separator (S-301)

In this separator, all light components other than acrylic acid and water exit in Stream 6. The acrylic acid and water are partitioned between Streams 6 and 7 according to Raoult's law. For acrylic acid, the vapor-pressure relationship is:

$$\ln P^*(\text{mm Hg}) = 19.776 - \frac{5450.06}{T(\text{K})} \qquad (3)$$

For this semester, you may assume that both the temperature and the pressure of this unit can be varied independently and at no cost.

Acrylic Acid Separator (S-302)

In this separator, assume that all acrylic acid exits in Stream 8, and all water exits in Stream 9. This means that the separator is behaving "perfectly." This is an approximation which we are using this semester but which may not be used in future semesters.

Assignment

Your assignment is to perform material balances on this process to determine the gross profit at different operating conditions. The gross profit is defined as:

$$\text{gross profit} = \text{value of products - cost of reactants} \qquad (4)$$

For this semester, the only product that has value is acrylic acid. The reactants are propylene and steam. The market prices for acrylic acid and propylene may be found in the *Chemical Marketing Reporter*, which may be found in the Evansdale library; for the former species, use the value for 99+% acrylic acid. The price for steam is $6.50/1000 kg. In your report, you should also discuss other expenses associated with acrylic acid production which are not included in the gross profit (Eq. 4) and how these additional expenses would affect the (actual) profit.

You should calculate material balances for the following cases:

Groups designated A: reactor at 200°C, 300°C, 400°C, 500°C, 600°C
Groups designated B: reactor at 250°C, 350°C, 450°C, 550°C, 650°C

Both groups should analyze their reactor cases for the following conditions in S-301:

Constant pressure of 1 atm: $T = 40°C$, 50°C, 60°C
Constant temperature of 50°C: $P = 1$ atm, 2 atm, 3 atm

The goal is to determine the optimum operating conditions, i.e., those yielding the maximum gross profit. The above cases must be done; however, you may run additional cases, at your discretion, by interpolating reactor performance data, or by moving outside the temperature and pressure range in S-301 to suggest more profitable operating conditions.

When reporting the results of all cases, graphs are superior to tables. You should plot graphs of gross profit vs. reactor temperature, with different curves on the same plot for different separator temperatures and pressures.

It is assumed that this problem will be solved either using a spreadsheet, a program like Mathcad, or by writing a computer program in Fortran or C. Solving this problem with only hand calculations is unacceptable.

Hint: Since it is easier to perform material balances from feed to product, choosing a feed basis and then scaling up to the desired acrylic acid production rate is recommended.

Other Information

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

The information in this document is considerably simplified, and consequently is valid for this project only. Unless specifically stated in class, you may not use information in this document for future projects. Additional information, *e.g.*, physical properties, may be found in standard references (Refs. 1, 2).

Groups

You should form your own groups immediately and inform Professor Dadyburjor of the membership of the groups. Groups should contain either 3 or 4 members. Anyone not able to join a group should contact Professor Dadyburjor immediately.

Deliverables

You must deliver a report prepared by a word processor and conforming to the document entitled *Written Design Reports* which you will receive. All graphs and tables must be generated by computer. It is your responsibility to keep sufficient back-up copies of your work. Computer failure, hard-disk failure, a corrupted floppy disk, *etc.*, are not necessarily excuses for a penalty-free extension. The report is due on December 1, 1997 at 4:45 p.m. Late reports will be penalized one grade per day.

The appendix to your report should contain sample spreadsheets or computer programs. The appendix should also contain a set of detailed hand calculations for your optimum case, to prove the validity of your computer calculations.

Revisions

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 edition*, Wiley, New York (1986).

2. Perry, R.H. and D. Green, eds., *Perry's Chemical Engineering Handbook, 6th edition*, McGraw-Hill, New York (1984).