Material Balances
Design Problem Statement
Production of Acetone

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 [1]. 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 50,000 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.

Process Description

Figure 1 is a flow diagram of a simplified process for acetone 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, an aqueous solution of isopropyl alcohol is fed into the reactor, where the stream is vaporized and reacted over a solid catalyst at 2 atm. The reactions occurring within the reactor are as follows:

$CH_3\text{-}CHOH\text{-}CH_3 \rightarrow CH_3\text{-}CO\text{-}CH_3 + H_2$ (1)
isopropyl alcohol (IP) acetone (AC) hydrogen (HY)

$2\ CH_3\text{-}CHOH\text{-}CH_3 \rightarrow (CH_3)_2CH\text{-}O\text{-}CH(CH_3)_2 + H_2O$ (2)
2 IP di-isopropyl ether (DE) water (WA)

$CH_3\text{-}CHOH\text{-}CH_3 \rightarrow CH_2{=}CH\text{-}CH_3 + H_2O$ (3)
IP propylene (PY) WA

Eq. (1) is the desired (AC-production) reaction. Eq. (2) is a condensation reaction (to DE) that is expected to be significant at lower temperatures, and Eq. (3) is a dehydration reaction (to PY) that is expected to be significant at higher temperatures. The outlet stream from the reactor is then passed through a scrubbing column. Here the vapor stream is contacted with liquid water, resulting in all the components except hydrogen and propylene being absorbed into the liquid phase. The vapor-phase outlet from the scrubber (HY and PY) may be separated and sold, or flared, depending on the economics. The liquid-phase outlet from the scrubber is passed to a light-gas separator, where the stream is flashed to a lower pressure and a different temperature, such that most of the WA, IP and DE, and some of the AC, form a liquid phase. The vapor phase from the light-gas separator

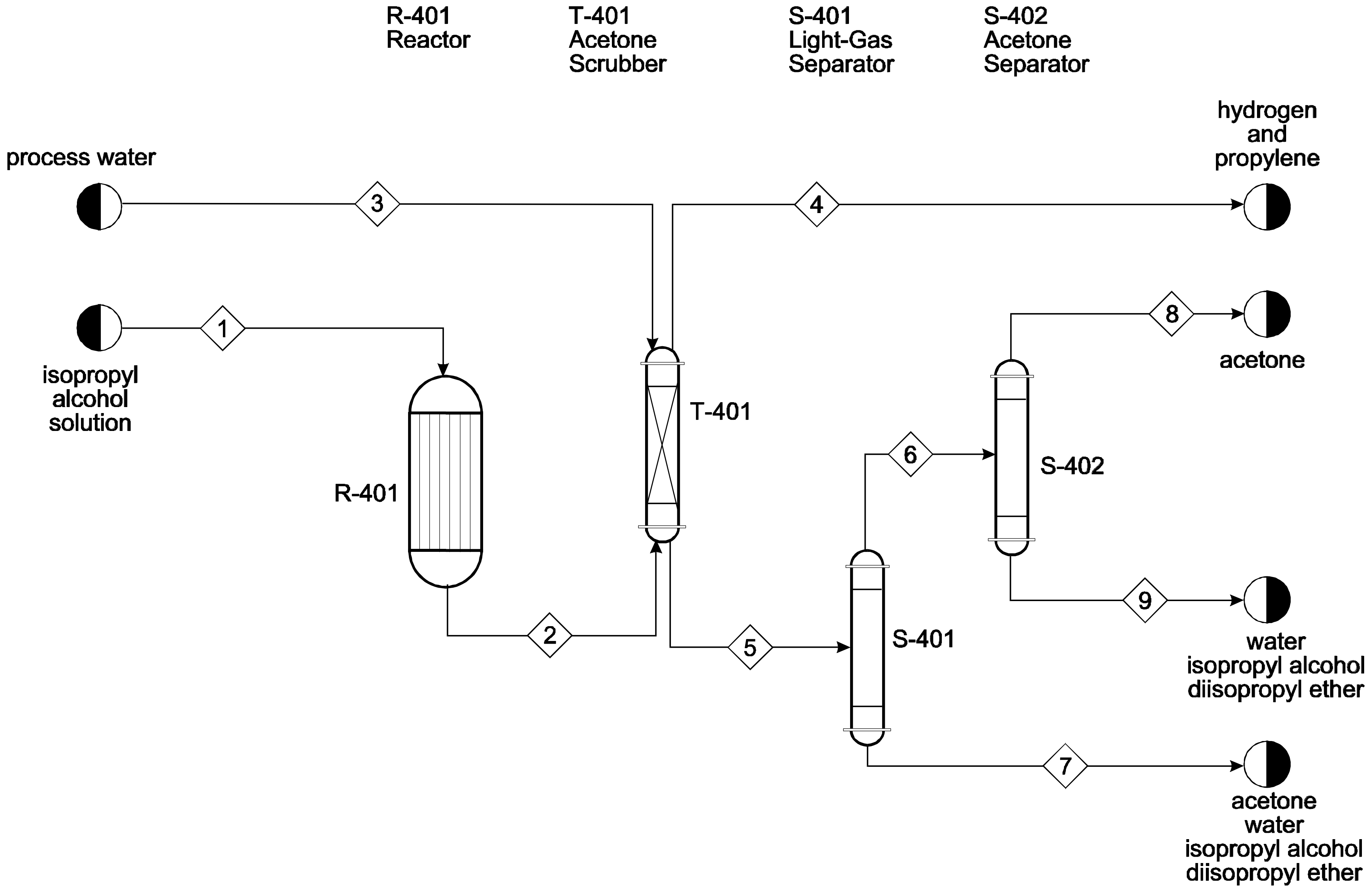

Figure 1: Process Flow Diagram for Acetone Production

consists of most of the AC and some of the WA, IP and DE. This stream is separated in an acetone separation unit such that pure AC leaves as one stream (the main product stream). The other stream from the distillation column is considered as a waste stream. The liquid phase from the light-gas separator is considered as the second waste stream.

Process Streams

Stream 1: This stream is an aqueous solution of IP containing 88 wt% IP and the balance WA. The stream is pumped into the reactor at 2 atm.

Stream 2: This vapor stream is the reactor effluent. It is at the reactor temperature and 2 atm.

Stream 3: This stream is process water, pumped to a pressure of 2 atm and a temperature of 30°C.

Stream 4: This vapor stream contains all of the PY and all of the HY entering the acetone scrubber. It is at the temperature and pressure of the scrubber (70°C, 2 atm). This stream may be either flared, or processed further and sold, depending upon the economics.

Stream 5: This liquid stream contains all of the AC, IP, DE and WA (including the process water in Stream 3) at the same temperature and pressure as Stream 4.

Stream 6: This vapor stream exiting the light-gas separator is at the temperature and pressure of the light-gas separator. The components in Stream 5 are partitioned between Streams 6 and 7 according to Raoult's law.

Stream 7: This is the liquid stream from the light-gas separator, at the temperature and pressure of the light-gas separator. In the present simplified design, this is considered a waste stream.

Stream 8: This liquid stream, a product of the acetone separation unit, contains pure acetone.

Stream 9: This liquid stream, the other product of the acetone separation unit, contains all of the other components from Stream 6, *viz*., WA, IPA and DE. In the present simplified design, this is considered a waste stream.

Process Units

Reactor (R-301)

In this reactor, the reactions in Eqs. (1) - (3) occur. The conversion of IP and the selectivities of DE and PY, each relative to AC, at various temperatures are given in Table 1. These values are for the reactor operating pressure of 2 atm. For this semester, you may assume that the temperature of R-301 can be varied at no cost.

Table 1
Selectivity and Conversion at Different Temperatures

Temperature (°C)	Conversion (%)	DE Selectivity (moles DE / moles AC)	PY Selectivity (moles PY / moles AC)
300	46.3	0.0100	0.08
310	55.4	0.0095	0.09
320	64.6	0.0090	0.10
330	73.4	0.0080	0.11
340	81.3	0.0070	0.12
350	87.8	0.0060	0.13
360	92.7	0.0050	0.14
370	96.1	0.0040	0.15
380	98.2	0.0030	0.16
390	99.2	0.0020	0.17
400	99.7	0.0010	0.18

Acetone Scrubber (T-401)

This piece of equipment is a column filled with packing material. Liquid water flows down the column (as Stream 3), and the vapor-phase Stream 2 from the reactor flows up. For the present level of design, assume that the ratio of the molar flow rates of WA in Stream 3 to AC in Stream 2 has the value of 0.01. In addition, you may assume that all of the HY and all of the PY remain in the vapor phase and exit the unit as Stream 4, and the balance exits as a liquid in Stream 5. The temperature of the exit streams is assumed to be 70°C; further assume that these temperatures may be maintained at no cost, independent of the reactor temperature, the temperature of Stream 2.

Light-Gas Separator (S-401)

In this separator, the pressure is quickly reduced to a constant value of 0.5 atm, resulting in the components of Stream 5 being partitioned between Streams 6 and 7. Assume that this flash occurs according to Raoult's Law. For acetone, use the constants for the Antoine equation as given in Table 6.1-1 of Ref. [2]. Relations between the vapor pressure of other components and the temperature are of the form:

$$\ln_e P_i^* \,[\text{mm Hg}] = A_i - \frac{B_i}{T\,[\text{K}] + C_i}$$

with the constants A_i, B_i and C_i having the values provided in Table 2 below.

Table 2
Values of Constants in Eq (4) [3]

Component i	A_i	B_i	C_i
IP	18.6929	3640.20	-53.54
DE	16.3417	2895.73	-43.15
WA	18.3036	3816.44	-46.13

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

Acetone Separation Unit (S-402)

In this separator, assume that all acetone exits in Stream 8, and all the other products (IP, WA, DE) exit 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 obtain the optimum design conditions for the process as described, by carrying out the appropriate material balances. Here the optimum refers to a "gross profit," defined as:

$$\text{gross profit} = \text{value of products} - \text{cost of materials input} \tag{5}$$

For this semester, the products of value are acetone, and perhaps Stream 4. Do not take credit for any of the waste liquid streams. The materials input to the process are the aqueous IP solution and process water. The market prices for the aqueous IP solution and for the pure acetone may be found in *The Chemical Marketing Reporter (CMP)*, available in the Evansdale library. (For the aqueous IP solution, use the value for the aqueous solution with IP concentration closest to 88 wt%.) The price for process water is \$0.04/1000 kg. The value of Stream 4 is to be calculated using the following approximation:

$$V_4 = 1.42\, y_{HY} + 13.17\, y_{PY} - S_{HP}\, y_{HY}\, y_{PY} \tag{6a}$$

Here y_i represents the mole fraction of component i in Stream 4. Parameter V_4 is the value of Stream 4, in [\$/kmol]. The parameter S_{HP} represents the cost of separating HY and PY; use the following value:

$$S_{HP} = 27.00 \text{ [\$/kmol]} \tag{6b}$$

If the value of Stream 4 is found to be positive in Eq. (6a), then that value should be included in Eq. (5). If the value of Stream 4 is negative, then assume that it costs more to separate the components of Stream 4 than the pure components are worth. In that case, Stream 4 should be simply flared, at zero cost and zero benefit, so the value of that stream is zero in Eq. (5).

You should calculate material balances for the following cases:

Odd-numbered groups: reactor at 300°C, 320°C, 340°C, 360°C, 380°C, 400°C
Even-numbered groups: reactor at 310°C, 330°C, 350°C, 370°C, 390°C, 400°C

Use the following conditions in S-401 for each reactor case:

Constant pressure of 0.5 atm: T = 60°C, 61°C, 62°C, 63°C, 64°C, 65°C

Since it is easier to perform material balances from feed to product, it is recommended that you choose a feed basis and then scale up to the desired acetone production rate. However, note that the optimum conditions should be picked on the basis of a <u>constant production rate of acetone</u> in Stream 8, rather than a constant feed rate in Stream 1. In other words, you should select the optimum <u>after</u> scale up, not before.

As mentioned above, the goal is to determine the optimum operating conditions, i.e., those yielding the maximum gross profit. While all the above cases of process conditions must be run and considered in the search for the optimum, you may run additional cases, at your discretion, to suggest more profitable operating conditions. These cases may be obtained, say, by interpolating reactor performance data, or by moving outside the temperature and pressure range in S-301. These additional cases should also be detailed in your report.

Because of the simplifications of the process used here, it is possible that the gross profit may be negative, even for the optimum process conditions. In your report, you should discuss qualitatively some ways in which the process could be altered to increase the gross profit. You should also discuss other expenses associated with acetone production which are not included in the gross profit (Eq. 4) and indicate how these additional expenses would affect the (actual) profit.

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.

It is assumed that this problem will be solved by using a spreadsheet, or a program like Mathcad, or by writing a computer program in Fortran or C. Sample spreadsheets or computer programs must be included in the Appendix to your report. Solving this problem with <u>only</u> hand calculations is unacceptable. However, verify your optimum case by carrying out one set of hand calculations, and include these as an Appendix to your report.

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 [2-4].

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 7, 1998 at 4:45 p.m. Late reports will be penalized 10 percent of the maximum points per day.

An Appendix to your report should contain sample spreadsheets or computer programs. Another Appendix should 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. 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.