Material Balances
Design Project
Manufacture of Diethyl Ether

Diethyl ether (DEE) is a colorless, highly volatile, flammable liquid with a characteristic odor. It is an important solvent in the production of cellulose acetate and other cellulose-based polymers. Other uses for DEE are as a starter fluid for diesel and gasoline engines, and as a solvent for Grignard and other reactions involving organometallic reagents. Previously, it was used as a general anesthetic.

The common production method for DEE is as a by-product from the vapor-phase hydration of ethylene to make ethanol. However, we have an excess of ethanol in our facility. Therefore, the process of interest in this assignment uses the vapor-phase dehydration of ethanol.

The assignment is to evaluate a process to manufacture 80,000 metric tons/year of a liquid containing at least 99.5 mol% DEE, subject to constraints which will be defined later in this document.

A suggested process flow diagram (PFD) of the unit, termed Unit 1200, is attached as Figure 1. You should use this as a starting point. However, any change that you can justify on economic grounds (and that does not violate the laws of nature) is not only allowed but encouraged. Your assignment is to develop an optimum case based upon an objective function, to be defined later. It is your job to define the decision variables, and to choose and implement a method to arrive at an optimum design.

Process Description

See Figure 1. The fresh feed to the unit, Stream 1, consists of 70 mol% ethanol in water. This stream is pumped from storage and sent to an on-site feed vessel, V-1201, where it is mixed with recycled ethanol, Stream 8. The stream leaving V-1201, Stream 2, reacted in the reactor, R-1201. The reactor contains a packed bed of alumina catalyst. The main reaction is:

$$\underset{ethanol}{2C_2H_5OH} \rightarrow \underset{DEE}{(C_2H_5)_2O} + H_2O \tag{1}$$

The only side reaction that occurs in R-1201 is the dehydration of DEE to form ethylene:

$$\underset{DEE}{(C_2H_5)_2O} \rightarrow H_2O + \underset{ethylene}{2C_2H_4} \tag{2}$$

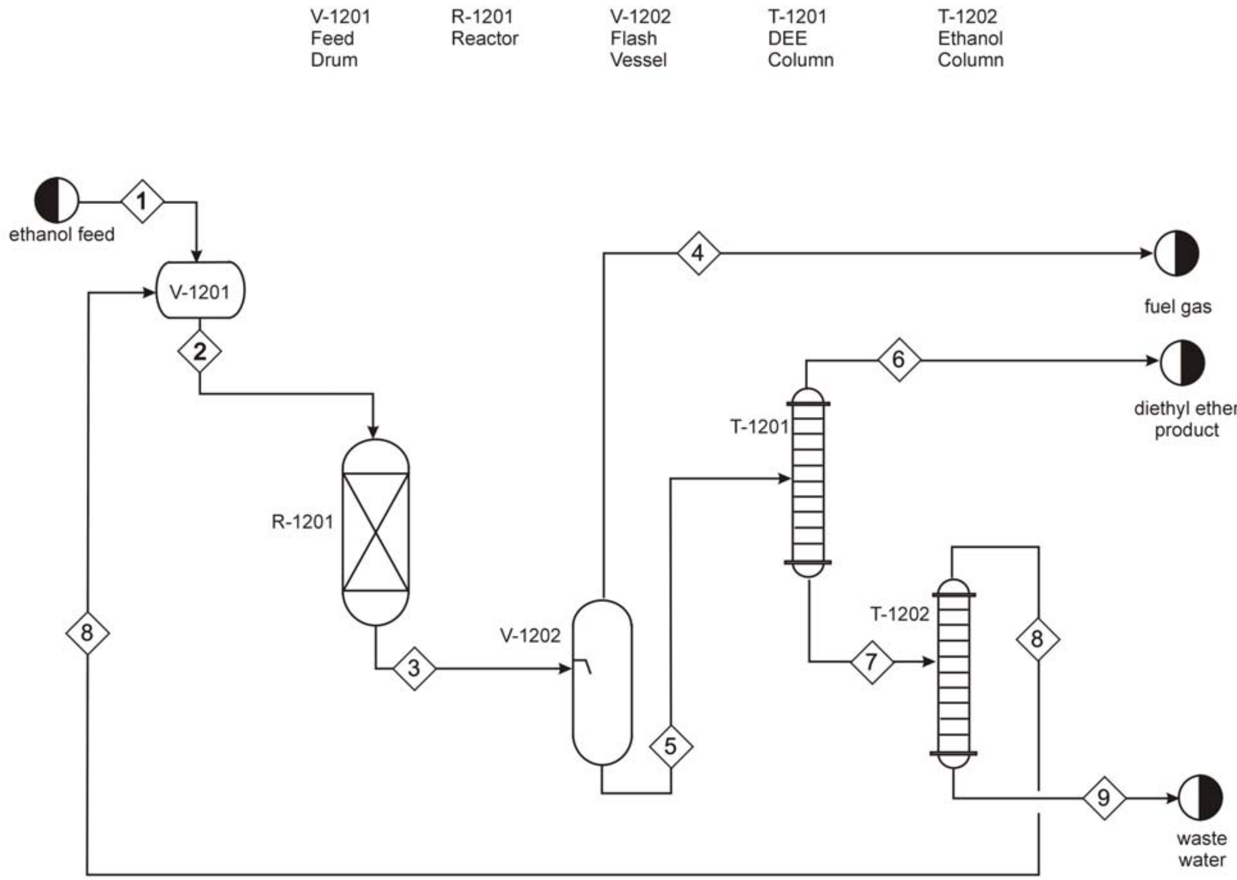

Figure 1: Unit 1200 Diethyl Ether Process

The reactor effluent, Stream 3, contains ethylene, unreacted ethanol, DEE, and water. Stream 3 is fed to a flash vessel, where it may be assumed that all ethylene enters Stream 4, while all other components enter Stream 5. The contents of Stream 4 have no value. Stream 5 is sent to a distillation column, T-1201, where at least 99% of the DEE is recovered as product in Stream 6 at 99.5% purity, and it may be assumed that all of the waters enter Stream 7. In T-1202, all of the DEE enters the recycle stream, Stream 8, and that the composition of Stream 8 is 95 wt% ethanol in water, if the DEE is ignored. The waste water stream, Stream 9, my contain no more than 1 wt% ethanol

Process Details

Feed Stream

Stream 1: Feed: liquid solution of 70 mol% EtOH in water.

Effluent Streams

Stream 4: Fuel Gas: light-gas stream of ethylene with traces of water vapor, DEE and EtOH in the vapor phase that can be ignored.

Stream 6: Product Liquid: contains at least 99.5 mol% DEE, with the balance being ethanol.

Stream 9: Wastewater: may contain no more than 1 wt% ethanol.

Recycle Stream.

Stream 8: Top product of T-1202, contains DEE, ethanol, and water.

Reactor

Only the reactions in Equations (1) and (2) are assumed to occur. The ranges of parameters that can be used are: temperature between 400-600 K and pressure between 1000-1500 kPa. The selectivity *S* for DEE formation in R-1201 is given in Table 1.

Table 1. Fractional Selectivity Data for DEE

Temperature *T* [K]	400	400	450	450	500	500	550	550	600	600
Pressure *P* [kPa]	1000	1500	1000	1500	1000	1500	1000	1500	1000	1500
Selectivity	24.87	21.48	12.60	10.84	7.43	6.38	4.94	4.23	3.59	3.08

$$S = \frac{\text{change in the molar flow rate of DEE}}{\text{change in the molar flow rate of ethylene}}$$

Economic Analysis

Objective Function

When evaluating alternative cases, the following objective function should be used. The gross profit (GP) is defined as:

GP = (value of product and by-product) - (feed cost) - (other operating costs) (8)

It is desirable to maximize the GP.

Raw Material Cost, Product Value

These are provided in Table 2. When using these numbers, you should be aware that they may be modified later, so write programs, spreadsheets, etc., with this in mind.

Table 2. Material Prices [1]

Component	DEE	Ethanol
Price [$/kg]	1.51	0.98

Waste treatment

For Stream 23 $5.00/1000 kg

Optimization

Other Information

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

During the actual process, the liquid formed in V-1202 separates into two phases, which must be added as two streams separately to T-1201. Further, DEE and water could form an azeotrope, a mixture which is difficult to separate by distillation. Finally, a peroxide inhibitor is generally added to the product DEE for safety reasons. These issues are not considered in this design project. Additionally, the selectivity data used may not correspond to the actual kinetics and equilibrium.

Groups

You will work on this project in groups of four. More details of group formation and peer evaluation will be discussed in class.

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. You are advised to start working on this problem as soon as possible, so that your questions may be asked, and clarifications made, sooner rather than later.

Deliverables

Written Report

Each group must deliver a word-processed report that is clear and concise and adheres to the prescribed format. The format is explained in the Written Report Guidelines, available at http://www.che.cemr.wvu.edu/publications/projects/index.php. A brief summary is provided here.

The body of the report should be short, emphasizing only the results and explaining why the results presented are optimal. The report must contain a labeled PFD and a stream table. The stream table must include temperature, pressure, phase, total mass flow rate, total molar flow rate, and component molar flow rates. When presenting results for different cases, graphs are often superior to tables (but see discussion in the Guidelines).

The report appendix should contain details of calculations. These calculations should be annotated so that they are easy to follow -- calculations that cannot be followed easily will lose credit. Computer output without detailed explanations is not appropriate; neatly hand-written calculations are best.

Reports not adhering to the prescribed format will receive significant deductions and may have to be rewritten.

The documents on the following Web site provide an indication of the expected attributes of a written design report: http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php.

The written report is due on Monday, December 5, 2011 by 3:00 pm.

References

1. http://www.icis.com/chemicals/channel-info-chemicals-a-z/