Dimethyl Ether Production
Material Balances

Dimethyl ether (DME) is used primarily as a propellant. It is miscible with most organic solvents and has high solubility with water. Recently, the use of DME as a fuel additive for diesel engines has been investigated due to its high volatility (desirable for cold starting) and high cetane number.

DME is produced by the catalytic dehydration of methanol over zeolite catalyst. The reaction is as follows:

$$2CH_3OH = CH_3OCH_3 + H_2O$$

In the temperature range of normal operations, there are no side reactions. A simplified process flow diagram for a DME process is shown in Figure 1.

Process Description

Fresh methanol, Stream 1, is combined with recycled reactant, Stream 8, and vaporized prior to being sent to a fixed bed reactor, operating between 250°C and 400°C. The single pass conversion in the reactor must be limited to 80% due to equipment constraints. The reactor effluent, Stream 4, is then cooled prior to being sent to the first of two distillation columns. DME product is taken overhead from the first column. The second column separates water from the unreacted methanol. The methanol is recycled back to the front end of the process, while the water is sent to waste treatment to remove trace amounts of organic compounds.

Reaction Information

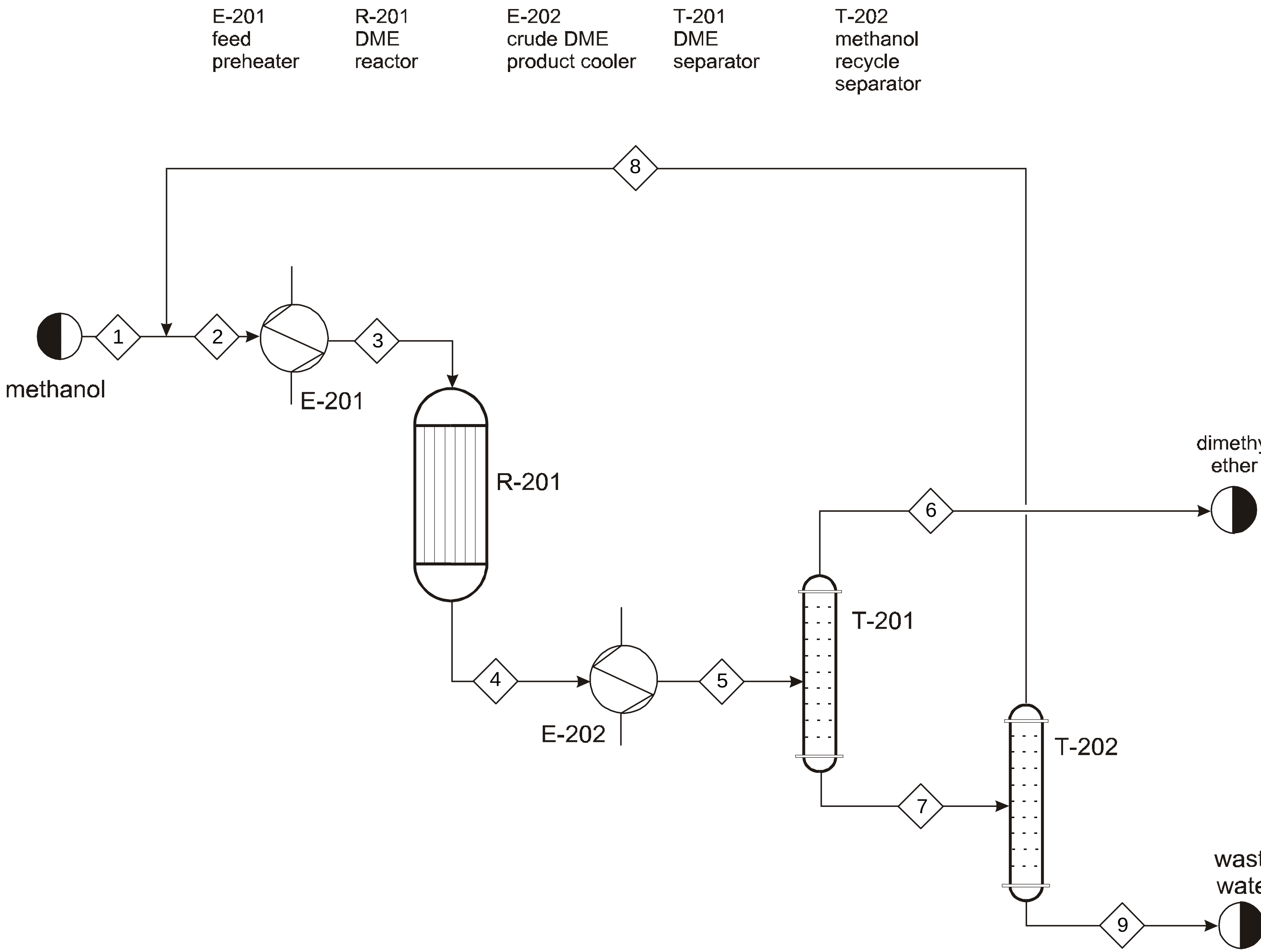
The reaction taking place is mildly exothermic with a standard heat of reaction of –11,770 J/mol. The equilibrium constant for this reaction at three different temperatures is given below:

T (K)	K_p
473 (200°C)	34.1
573 (300°C)	12.4
673 (400°C)	6.21

The equilibrium conversions for pure methanol feed over the 200°C-to-400°C range are all greater than 83%. By limiting conversions to 80%, the reaction will not be equilibrium limited.

Catalyst Information

The process uses a crystalline silicon-aluminum oxide catalyst, called a zeolite. This particular catalyst performs well in the 200°C-to-400°C range, but deactivates rapidly if heated



Unit 200 - Dimethyl Ether Process

above 400°C. The design given in Figure 1 uses a single, packed bed reactor. The reactor is insulated, with the result that heat produced by the exothermic reaction raises the catalyst temperature. At 80% conversion with fresh catalyst, the reaction temperature goes from 244°C at the inlet of the catalytic reactor to 364°C at the outlet.

Fractional Conversion of Methanol

An operating equation has been developed for this specific reactor relating fractional conversion of methanol to the outlet temperature of the reactor and the time that the catalyst has been on stream. This relationship is

$$\ln\left(\frac{f_m}{1-f_m}\right) = -\frac{4840}{T} - (3.0\times 10^{-5})(T-520)t + 8.9370$$

when the flowrate of Stream 3 = 400 kmol/h and

f_m = fractional conversion of methanol,
T = reactor outlet temperature in K, and
t = catalyst time on stream in days.

Operating Costs

Information on operating costs will be provided in a subsequent memo.

Problem

You, the engineering team, are to plan the operation of the DME process in order to produce 50,000 metric-tons/y (50,000,000 kg/y) to meet a contract with another company. Your goal is to minimize operating costs and maximize profit. You are constrained by the reactor feed rate (Stream 3 = 400 kmo/h), 80% fractional conversion of methanol, 400°C maximum outlet temperature, and operating costs. Details on operating costs and the anticipated costs for the feedstock and product will be provided in a subsequent memo.

You may not use CAD software but are encouraged to use spreadsheet calculations. You may write your own program if you prefer. If you write a program, any programming language is acceptable. Whether you use a spreadsheet or program, you must turn in hand calculations for one case to demonstrate that the program or spreadsheet is written correctly.

Group Formation

A design group is to consist of at least three but no more than four members. No other combinations are acceptable. You are free to make groups by yourselves. When you have formed a group, please write the names of group members on the chart posted on Dr. Kugler's door. Individuals not in groups by November 13 will be assigned to groups.

Reports

Each group will be expected to prepare a written report recommending the best operating procedures for the DME process. This report is due at 3:00 PM, Wednesday, December 6. The report should follow the Department's design-report guidelines. Data should be in the form of graphs and tables since this serves both to condense results and make them easily understandable. The appendix should include your spreadsheet or computer program and a hand calculation of a representative case.

Report Authors

Although work on a group report can never be divided equally, only those members making substantial contributions to the final report should be listed as authors.

E. L. Kugler
November 6, 2000

Supplemental Information for Dimethyl Ether Material Balance Project

Feed and Product Prices

methanol	\$ 0.60 per gallon
dimethyl ether	\$ 0.43 per pound

Other Costs

The operating costs for dimethyl ether production are related to temperature. High temperature operation requires that the feedstock be heated to high temperature, then cooled from high temperature to an unspecified low temperature where the dimethyl ether, methanol, and water condense. Other costs include operation of the distillation columns, labor costs, etc. For this project, all operating costs are described by the following function related to temperature.

$$\text{operating costs(\$/lb of } CH_3OH \text{ in Stream 2)} = 0.052 + 0.00020(T\text{-}523)$$

where T is the temperature in K.

Catalyst Deactivation Function

The equation relating temperature and fractional conversion includes a catalyst aging function. This function remembers catalyst history. The function has the form

$$\text{catalyst aging function} = -(3.0 \quad 10^{-5})(T\text{-}520)\text{t}$$

where T is temperature in K and t is time in days. Look at the following examples to see how the function works.

<u>Case 1</u> If the catalyst has been run for the first 60 days at 620 K,

$$\text{catalyst aging function (Case 1)} = -\ (3.0 \quad 10^{-5})(620\text{-}520)(60)$$

<u>Case 2</u> However, if the catalyst was run 40 days at 600 K followed by 20 days at 620 K,

$$\text{catalyst aging function (Case 2)} = -\ (3.0 \quad 10^{-5})(600\text{-}520)(40) - (3.0 \quad 10^{-5})(620\text{-}520)(20)$$

Catalyst Replacement

The catalyst may be replaced with fresh catalyst. New catalyst costs \$100,000 and requires 5 days of operating time for installation and startup.

11/08/2000