ChE 456
Spring 2004
Major 2

MTBE Production

Despite the uncertain future of MTBE as a gasoline additive, we have developed new, proprietary catalyst technology for the MTBE synthesis reaction. Existing plants have been retrofitted for this technology, such as the facility you studied previously; however, we do not have an optimized, grass-roots design of a facility using this proprietary technology. We are also working on other uses for MTBE. Therefore, we would like to have a process design available so, if the market for MTBE expands, we are in a position to move quickly.

Therefore, your assignment is to design a grass-roots process that produces 100,000 tonne/y of MTBE. The facility is to manufacture MTBE from methanol and isobutylene. Isobutylene is obtained from a refinery cut, and it also contains 1-butene and 2-butene, both of which do not react with methanol. Depending on where a future facility would be built, there are two possible sources of isobutylene. These are shown in Table 1. Part of your assignment is to recommend the better location to build a plant based on the locally available raw material.

Table 1: Possible Raw Material Feeds (mass %)

	Isobutene	1-butene	2-butene
Refinery Feed #1	23	10	67
Refinery Feed #2	40	35	25

Economic Parameters

- Optimization of the process should be carried out using the net present value, NPV, as the objective function
- The design should be for a new, grass-roots facility.
- Land costs are negligible.
- Taxation rates are 40% per year.
- Five-year MACRS depreciation of capital investment should be used.
- An interest (hurdle) rate for this project is 12% after taxes.
- The project length is 10 years after start up, which occurs at the beginning of year 3.
- There is no salvage value
- Working capital is 6 months supply of raw materials + 6 months of labor costs.
- Construction period is 2 years with a distribution of fixed capital investment as 60%, 40% at the ends of years 1, 2, respectively.
- The cost of the feed is the cost of the butanes not returned to the refinery (either in a mixture or in a mostly pure stream), based on the cost of pure isobutene. You may assume that whatever amount of butenes is needed can be supplied by the refinery.

Process Design Parameters

- The following specifications for the product must be met:
  MTBE – purity >95 mass% and less than 0.1% water
- Any liquid organic stream may be burned in a fired heater as fuel, and a credit may be taken for the fuel value (LHV) of the stream.
- All distillation columns must be simulated using rigorous unit operations (either TOWR or SCDS in Chemcad). Failure to use rigorous algorithms in the final case will result is a loss of credit. Preliminary screening using short-cut methods is acceptable.
- Butenes returned to the refinery must be 99.5 mass% pure.

Report Format

This report should be comprehensive and should conform to the guidelines. It should be bound in a folder that is not oversized relative to the number of pages in the report. Figures and tables should be included as appropriate. An appendix should be attached that includes items such as Chemcad output and sample calculations. These calculations should be easy to follow. The confidentiality statement should be the very last page of the report.

The written report is a very important part of the assignment. Reports that do not conform to the guidelines will receive severe deductions and will have to be rewritten to receive credit. Poorly written and/or organized written reports may also require re-writing. Be sure to follow the format outlined in the guidelines for written reports.

The following information, at a minimum, must appear in the main body of the final report:

1. a computer-generated PFD (not a Chemcad PFD) for the recommended optimum case,

2. a stream table containing the usual items,

3. a list of new equipment for the process, including bare module and installed costs, plus equipment specifications (presented with a reasonable number of significant figures),

4. a summary table of all utilities used,

5. a clear summary of alternatives considered and a discussion, supported with figures, of why the chosen alternative is superior,

6. a clear economic analysis which justifies the recommended case

7. a Chemcad report only for your optimized case (in the Appendix). This must contain the equipment connectivity thermodynamics, and overall material balance cover pages, stream flows, equipment summaries, tower profiles, and tray design specifications (if you use Chemcad to design the trays). It should not contain stream properties. Missing Chemcad output will not be requested; one letter grade will be deducted if the information is missing.

Oral Presentation

You will be expected to present and defend your results some time between February 21, 2005 and March 2, 2005. Your presentation should be 15-20 minutes, followed by about a 30-minute question and answer period. Make certain that you prepare for this presentation since it is an important part of your assignment. You should bring at least one hard copy of your slides to the presentation and hand it out before beginning the presentation.

Other Rules

You may not discuss this major with anyone other than the instructors. Discussion, collaboration, or any other interaction with anyone other than the instructors is prohibited. Violators will be subject to the penalties and procedures outlined in the University Procedures for Handling Academic Dishonesty Cases (begins on p. 47 of both the 2001-03 and 2003-05 Undergraduate Catalogs).

Consulting is available from the instructors. Chemcad consulting, *i.e.*, questions on how to use Chemcad, not how to interpret results, is unlimited and free, but only from the instructors. Each individual may receive five free minutes of consulting from the instructors. After five minutes of consulting, the rate is 2.5 points deducted for 15 minutes or any fraction of 15 minutes, on a cumulative basis. The initial 15-minute period includes the 5 minutes of free consulting.

Late Reports

Late reports are unacceptable. The following severe penalties will apply:

- late report on due date before noon: one letter grade (10 points)
- late report after noon on due date: two letter grades (20 points)
- late report one day late: three letter grades (30 points)
- each additional day late: 10 additional points per day

Appendix 1
Reaction Kinetics

The reactions and reaction kinetics are as follows:

$$CH_3OH + (CH_3)_2C = CH_2 \underset{\leftarrow}{\longrightarrow} (CH_3)_3C - O - CH_3 \tag{1}$$

$$-r = k_f \frac{C_{isobutylene}}{C_{methanol}} - k_r \frac{C_{MTBE}}{C_{methanol}^2} \tag{2}$$

where

$$k_f = 6.05 \times 10^{16} \exp\left(-\frac{85,400}{RT}\right) \tag{3}$$

$$k_r = 1.464 \times 10^{22} \exp\left(-\frac{129,600}{RT}\right) \tag{4}$$

The units of reaction rate, r_i, are mol/m^{3}h, and the activation energy is in J/mol. These kinetics are only valid when at least 20% excess methanol is present in the reactor feed stream.

Appendix 2
Chemcad Hints

Here are some Chemcad hints.

Use PSRK for the *K*-value and SRK for the enthalpy. However, for any absorber involving water and methanol, ideal vapor pressure for the *K*-value. You may also use ideal vapor pressure to simulate the MTBE purification tower.

For the reactor, make sure that you set the flag for a liquid-phase reaction and that the local reactor units correspond to those for the given kinetics.

For 2-butene, use trans-2-butene.