ChE 456
Spring 2004
Major 2

Production of Maleic Anhydride from Benzene

Problem Background

Following your preliminary report on the feasibility of the design of a 20,000 tonne/yr maleic anhydride plant using benzene as the feedstock, TSC, Inc.'s, client has decided to commission a further study. The purpose of this study is to assess the economic feasibility of an optimized process. Your design must include the final purification of the products as well as the front-end reaction and separation units, which were the focus of the previous project (Major 1). You are free to use the results of the previous study, and you may want to use them as a base case for starting this project.

For the current study, the following constraints apply:

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.
- The cost of operating labor is considerably lower than in the U.S., and a cost of $17,500 per operator per year should be charged.
- Land costs are negligible.
- Taxation rates are 22% per year.
- Straight-line depreciation of capital investment over a period of 5 years may be applied.
- An interest (hurdle) rate for this project is 10% 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 3 years with a distribution of fixed capital investment as 50%, 30%, 20%, at the ends of years 0, 1, and 2, , respectively.

Process Design Parameters

- No excess steam can be exported from the plant. Therefore, any steam generated within the process must be used within the process.
- The following specifications for products must be met:
    - Maleic Anhydride – purity >99.8 mass%
    - Quinone – purity > 99 mass%

    - Maleic Acid – purity > 99.8 mass%
- 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.
- The ideal vapor pressure *K*-value and latent heat Enthalpy options should be used for the Chemcad simulation.

In performing your study, you may wish to consider the following suggestions regarding the optimization.

Process Design Hints

- For the maleic anhydride process to have any chance of being profitable, the integration of process energy must be carefully planned. It is suggested that your study include a detailed heat exchange network design.
- In order to limit excessive reboiler and condenser duties on towers, the recycle flowrate of dibutylphthalate solvent should be limited. In addition, the severe recovery and purification specifications of this solvent should be carefully evaluated. For example, in Major 1, the purity of the solvent leaving the bottom of tower, T-502 was > 0.9999. If this purity specification is relaxed, to say 0.99, then the duty of the reboiler for T-502 is greatly reduced.
- For the by-products (quinone and maleic acid), the option of not purifying them but using them for fuel credit should be considered. An incremental comparison between the cost of separation and the loss in revenue from pure by-products should be used to determine the optimal strategy.

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; credit will be deducted as if the information is missing.

Oral Presentation

You will be expected to present and defend your results some time between February 23, 2004 and February 26, 2004. 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 the same as given in the first assignment and are repeated below:

$$\underset{\text{benzene}}{C_6H_6(g)} + 4.5O_2(g) \xrightarrow{k_1} \underset{\text{maleic anhydride}}{C_4H_2O_3(g)} + 2CO_2(g) + 2H_2O(g) \tag{A.1}$$

$$\underset{\text{benzene}}{C_6H_6(g)} + 7.5O_2(g) \xrightarrow{k_2} 6CO_2(g) + 3H_2O(g) \tag{A.2}$$

$$\underset{\text{maleic anhydride}}{C_4H_2O_3(g)} + 3O_2(g) \xrightarrow{k_3} 4CO_2(g) + H_2O(g) \tag{A.3}$$

$$\underset{\text{benzene}}{C_6H_6(g)} + 1.5O_2(g) \xrightarrow{k_4} \underset{\text{quinone}}{C_6H_4O_2(g)} + H_2O(g) \tag{A.4}$$

where

$$-r_i = k_i C_{benzene} \text{ or } -r_3 = k_3 C_{maleic\ anhydride} \tag{A.5}$$

and

$$k_1 = 7.7\times10^6 \exp(-25{,}143/RT) \tag{A.6}$$

$$k_2 = 6.31\times10^7 \exp(-29{,}850/RT) \tag{A.7}$$

$$k_3 = 2.33\times10^4 \exp(-21{,}429/RT) \tag{A.8}$$

$$k_4 = 7.20\times10^5 \exp(-27{,}149/RT) \tag{A.9}$$

The units of reaction rate, r_i, are kmol/m^3(reactor)s, the activation energy is given in cal/mol (which is equivalent to kcal/kmol), the units of k_i are m^3(gas)/m^3 (reactor)s, and the units of concentration are kmol/m^3(gas).

The catalyst is a mixture of vanadium and molybdenum oxides on an inert support. Typical inlet reaction temperatures are in the range of 350-400°C. The catalyst is placed in 25 mm diameter tubes that are 3.2 m long. The catalyst pellet diameter is 5 mm. The maximum temperature that the catalyst can be exposed to without causing irreversible damage (sintering) is 650°C.

For the fluidized bed reactor, you should use the same catalyst size and assume a particle density of 1200 kg/m^3. In a packed bed, the void fraction of the bed is 0.5.

Appendix 2
Chemcad Hints

In order to simulate the temperature spike in the reactor, the reactor is simulated as a co-current, packed bed kinetic reactor, with a molten salt stream as the utility. The kinetics given in Appendix A are used in the simulation.

For the simulation of the reactor as a fluidized bed, the reactor should be modeled as an isothermal plug flow reactor with 10% of the feed bypassing the reactor. This simulation is necessary to capture the isothermal nature of the fluidized bed but also to take into account the fact that the reactor feed bypasses the catalyst in the form of bubbles.

As with the previous project, any water absorbed in T-501 will react with maleic anhydride to produce maleic acid. The simulation of this reaction should be done in the same way as in Major 1.

Appendix 3
Raw Material Costs

Chemical	Price/Cost, $/kg
Dibutylphthalate	1.72
Benzene	0.45
Maleic Anhydride	0.93
Maleic Acid	0.90
Quinone	0.70

For utility costs, use the values in Chapter 6 of *Analysis, Synthesis, and Design of Chemical Processes*, R. Turton, R.C. Bailie, W.B. Whiting, and J.A. Shaeiwitz, 2nd ed., Prentice-Hall, 2003.