Major 3 – Design of a New Process for the Production of Acetone via the Dehydration of Isopropanol

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Background

Your company, FlawlessDesigns, Inc., has been contacted by a new client to design a new, grassroots facility to produce 30,000 tonnes/yr (1 year = 8000 operating hours) of pharmaceutical-grade acetone (99.9 mol%) via the dehydration of isopropanol (IPA). The client has considerable experience in the development and commercial application of new catalysts. Specifically, they have developed a new catalyst for the dehydration of IPA that they claim can operate at temperatures between 170 - 250°C. This catalyst would allow operation of the reactor heating loop with high-pressure steam and, therefore, would eliminate the need for a fired heater. This catalyst is available in two forms: cylindrical pellets 12 mm in length and 6 mm in diameter and small near-spherical particles approximately 300 ㎜ in diameter. The former is suitable for use in packed-bed reactors, while the latter can be used in fluidized bed reactors. Reaction pathways, kinetics, and physical characteristics for this catalyst are given in the following sections. The choice of reactor type and configuration is left to you.

The overall configuration for this new design has not been set. The purpose of this project is to produce the design that maximizes the after-tax Net Present Value (NPV) of the new process under the following economic constraints.

Internal Hurdle Rate (after tax) = 9%
Cost of Land = $ 2 million
Salvage Value = 0
Working Capital = 20% of the Fixed Capital Investment (C_{GR})
Tax rate (including federal, state, and local taxes) = 48%
Construction Period = 2 years
Fixed Capital Investment to be paid in two equal amounts at the end of years 1 and 2.
Depreciation: use the MACRS method over a 5 year period with the following yearly depreciation allowances:

- Year 1 (after start-up) = 20.0 %
- Year 2 (after start-up) = 32.0 %
- Year 3 (after start-up) = 19.2 %
- Year 4 (after start-up) = 11.52 %
- Year 5 (after start-up) = 11.52 %
- Year 6 (after start-up) = 5.76 %

Plant life = 10 years after start-up

Reaction Kinetics

The main reaction for producing acetone is

$$(CH_3)_2CHOH \rightarrow (CH_3)_2CHO + H_2$$

isopropanol acetone

and the kinetics for this reaction are given below:

$$-r_{IPA} = k_1 C_{IPA} \qquad \frac{\text{mol IPA}}{\text{m}^3\text{catalyst}\cdot\text{s}}$$

where

$$k_1 = 1.76\times10^5 \exp\left[-\frac{60{,}000}{RT}\right] \qquad \frac{\text{m}^3\text{gas}}{\text{m}^3\text{catalyst}\cdot\text{s}}$$

$$C_{IPA} = \frac{\text{mol IPA}}{\text{m}^3\text{gas}}$$

Although, several side reactions are possible, none of them take place to any considerable extent. The activation energy in the kinetic expression above is in units of kJ/kmol.

Catalyst Information

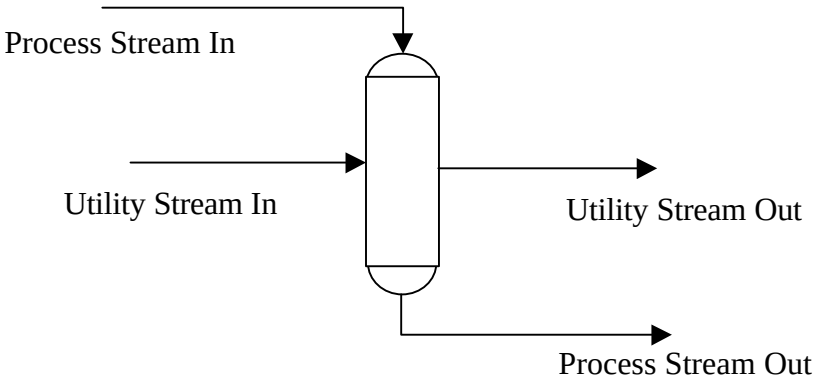
Catalyst physical properties are given below:

The density of the solid catalyst, ρ_s = 2500 kg/m^3 (both types of catalyst)
The packed bed voidage of the cylindrical pellets = 0.5
The voidage of the spherical particles at minimum fluidizing conditions = 0.45

Packed Bed Configuration

Tube diameter for catalyst tubes = 50 mm
Length of catalyst filled tubes = 20 ft (6.1 m)
Overall heat transfer coefficient from tubes to heating medium = 50 W/m^2°C
Installed cost of a shell and tube reactor = $ 3,000/m^2 of heat transfer surface
Bare module factor, C^o_{BM} = 2.5

Simulation of a packed bed reactor should be done using the kinetic reactor module in ChemCad using the countercurrent flow option for the utility stream. Option 5 should be used for the thermal mode. The appropriate ChemCad icon is given below. When this option is used, a temperature profile will be generated along the tubes of the bed. At no point should the temperature be outside the acceptable limits of 170 – 250°C.



Fluidized Bed Configuration

Tube diameter for in-bed heat exchange = 25 mm
Length of heat transfer tubes = 20 ft (6.1 m)
Overall heat transfer coefficient from tubes to heating medium = 200 W/m^2°C
Installed cost of a fluidized bed reactor = \$ 10,000 per m^2 of heat transfer surface
Bare module factor, C^o_{BM} = 2.5

The fluidized bed should be simulated using the Kinetic Reactor option in ChemCad and the isothermal plug flow option (thermal mode = 2) should be used. Due to the bubbling nature of the fluidized bed, a certain amount (assume 10%) of feed gas bypasses the catalyst. This means that the single-pass conversion of IPA can never exceed 90%. This means that 90% conversion can only be achieved in an infinite-sized reactor. Therefore, you must include a bypass when modeling this reactor on ChemCad. The operating temperature of the fluidized bed must lie within the operating range of the catalyst (170-250°C). The bed should be operated such that the superficial gas velocity at the conditions in the reactor lies in the range of 3 – 10 times the minimum fluidizing velocity (u_{mf}). The value of u_{mf} can be calculated using the Wen and Yu [1] correlation given in Equation (1) below:

$$\mathrm{Re}_{p,mf} = \frac{u_{mf} d_p \rho_g}{\mu_g} = [1135.69 + 0.0408 Ar]^{0.5} - 33.7 \qquad (1)$$

where

$$Ar = \text{Archimedes Number} = \frac{d_p^3 (\rho_s - \rho_g) \rho_g g}{\mu_g^2}$$

d_p = particle diameter

ρ_g = gas density

μ_g = gas viscosity

ρ_s = solid (catalyst) density

g = accelaeration due to gravity

Raw Material, Product, and Utility Costs

The cost of utility streams is given in Table 3.4 of your textbook [2]. You may assume that all steam pressures in Table 3.4 are available. In addition, cooling water, electricity, fuel gas, and refrigerated water (costed as "moderately low" refrigeration) are all available. The cost of treating wastewater should be taken as \$53/1000 m^3, and your design should produce wastewater with a maximum organic concentration of 0.1 wt% prior to treatment.

The cost of IPA and acetone are \$0.71/kg and \$0.92/kg respectively.

Thermodynamic Options and Models

For your ChemCad simulation of the process you should use the UNIQUAC K-value option and the SRK enthalpy option. Note that in the final ChemCad simulation, to be included in the appendix of the written report, all the columns must be simulated using a rigorous model, e.g., using TOWER or SCDS.

Base Case and Optimization

Although there is no base case available for the process with the new catalyst, a good starting point are the PFDs given in the first two projects and Figure B.3 in Appendix B of your textbook [2]. It is recommended, that as a first step in the solution of this problem, you establish a base case and perform an economic analysis. This will help you to determine the major cost areas and where to focus your attention during the optimization phase.

It is recommended that you do the flowsheet optimization using the Shortcut column option for the acetone purification tower. You can do the final rigorous simulation at the end, since the material balance for this column will not change during the optimization. Also, you should put a component separator in front of the acetone tower to remove the trace amounts of hydrogen in the liquid stream from the flash and absorber. This small amount of hydrogen will give Chemcad problems in the distillation section – so you must remove it.

Remember that you should spend most of you effort in optimizing the parts of the process that have a major economic impact on the NPV. You may wish to refer to Chapter 19 sections 19.1 and 19.2 of your textbook [2] for more information regarding optimization.

Report Specifications

The written report format should follow the guidelines for a full report given in Chapter 22 of your textbook [2]. An executive summary, not to exceed 4 double-spaced pages, should precede the report. The written report must contain at least the following information:

i. A PFD for your final (optimized) process
ii. A flow table containing information on all the major process streams given in the PFD. This information should include the temperature, pressure, phase, total mass and mole

flowrate, and component mole flowrates. All major process streams must be identified on the PFD and the flow table.

iii. An equipment summary table giving the details of all major equipment shown on the PFD.
iv. A table or tables giving a breakdown of the economics of the optimized process.
v. An appendix containing sample calculations for all relevant calculations. A table of contents should be given on the first page of the Appendix.
vi. A ChemCad report for final, optimized case must be given in the Appendix.
vii. A signed copy of the confidentiality statement must be provided as the last page of the report.

The written report is due in four weeks.

The oral presentations will be scheduled during the week that the written reports are due. You are expected to present your findings formally for 15 – 20 minutes and answer questions for the remainder of the 50 – 55 minute period. You are also required to bring at least one hard copy of your overheads to the oral. These will be returned to you with your written report after grading.

References

1. Wen, C.Y., and Y.H. Yu, *AIChE J*., **12**, 610 (1966).
2. 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.