Material Balances Project
Ammonia Production

Background

You work for a consulting company that has been hired to determine the most profitable operating conditions for an ammonia synthesis loop at your client's facility. You are only to evaluate the ammonia synthesis portion of a much larger process that takes coal, converts it into a synthesis gas (carbon monoxide and hydrogen), adds nitrogen and removes the carbon monoxide, adjusts the composition and produces ammonia. Ammonia is one of the five most produced chemicals in the industry. It is a raw material for nitrogen oxides and fertilizers, among others. The process in question is to produce 50,000 tonne/y of ammonia in an 8000-hour year.

Ammonia Production

Unit 600 produces ammonia from a feed mixture that contains stochiometric amounts of nitrogen and hydrogen plus inert gas that is nearly all methane. Figure 1 illustrates the main units in your client's design.

The composition of fresh feed is 24.5% nitrogen, 73.5% hydrogen and 2.0% methane. The methane is inert and does not react. The feed is compressed, mixed with the recycle stream, preheated and sent to the reactor. The reaction is equilibrium limited, which means that the reactor temperature limits the extent of reaction. The reaction and equilibrium constant, in the range of 700 K – 750 K are:

$$N_2 + 3H_2 = 2NH_3 \tag{1}$$

$$K = \frac{P_{NH_3}^2}{P_{N_2}^1 P_{H_2}^3} = 1.054 \times 10^{-12} \exp\left[\frac{12711}{T}\right] \tag{2}$$

where the units of K are atm^{-2} and T is in Kelvin. The reactor effluent is cooled and separated in a flash vessel, producing liquid ammonia and light gases. To prevent methane from building up in the recycle stream, a fraction of the light gases goes to a purge stream, and the remaining light gases are compressed and recycled.

The ammonia synthesis loop can be operated over the pressure range of 10 to 150 atm, reactor temperatures of 420°C to 480°C and purge-to-recycle ratios of 1/10 to 1/100. To simplify the material balance calculations, you may assume that the recycle stream contains no ammonia and that the ammonia stream contains no dissolved gases. The range of operating conditions involve trade-offs. Higher pressures increase the equilibrium conversion but increase the cost of compressing the reaction gases; lower reactor temperatures increase equilibrium conversion but increase cost by requiring more cooling to remove heat from the exothermic reaction; smaller purge-to-recycle ratios loose less reaction gas from the recycle loop but increase cost since more gas must be compressed for recycle back to the reactor.

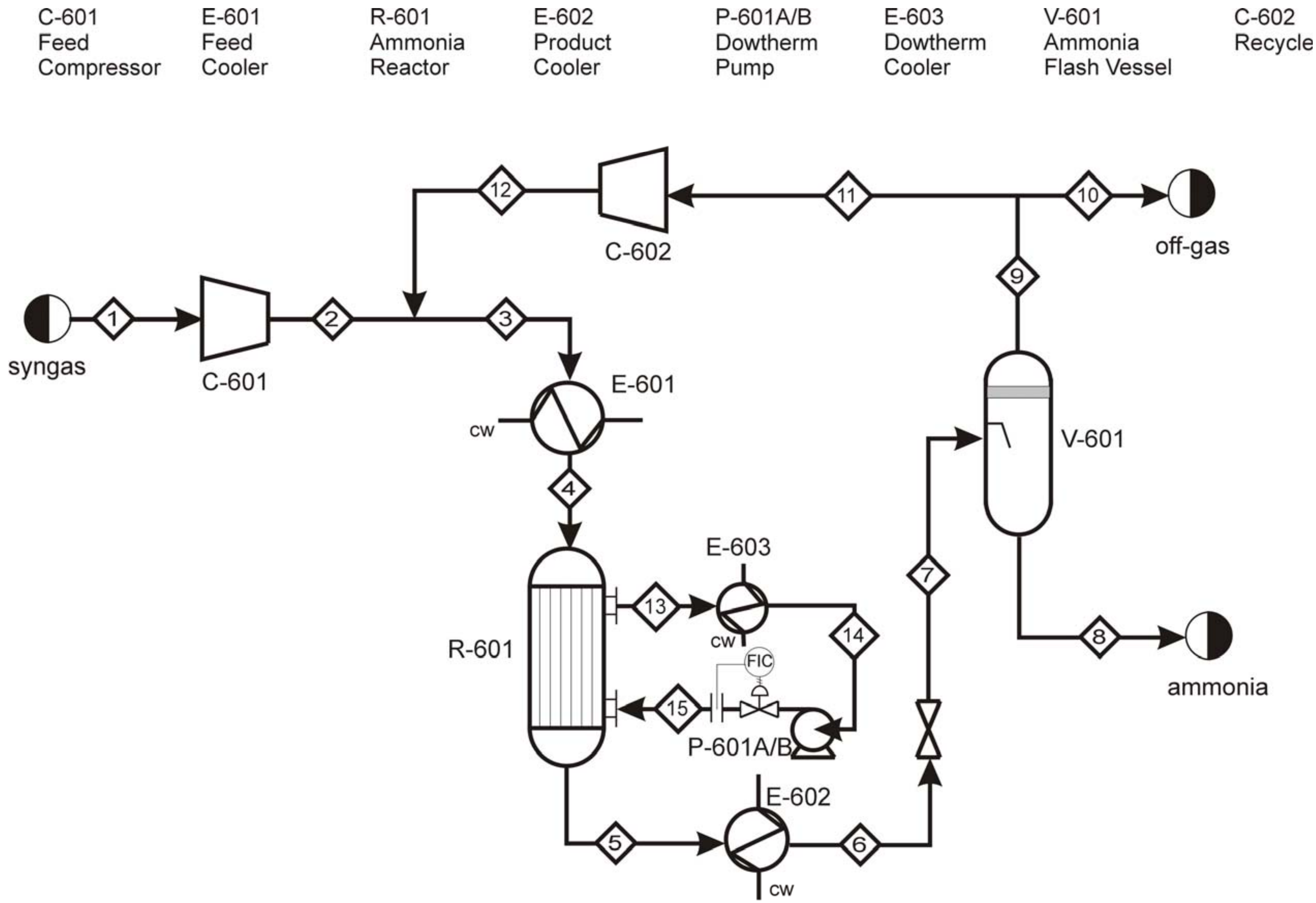

Figure 1: Ammonia Synthesis Loop

Problem

You, the engineering team, are to choose the best operating conditions for the ammonia synthesis process in order to produce 50,000 tonne/y (50,000,000 kg/y). Your goal is to minimize operating costs and maximize profit. You are constrained by the reactor temperature, reactor pressure, the purge-to-recycle ratio, and operating costs.

You may not use CAD software, but should use Excel spreadsheet calculations. Before developing a spreadsheet, you must solve the material balance by hand for at least one case to demonstrate that the spreadsheet is set-up correctly.

Group Formation

A student design group will consist of 4 group members. You are encouraged to choose a partner for this project to form a pair. When you have formed a pair, please write your names on the chart posted on Dr. Kugler's door. Dr. Kugler will combine pairs to form groups of four. Group assignments will be made on November 5.

Reports

Each group will be expected to prepare a written report recommending the best operating procedures for the ammonia synthesis process. This report is due at 3:00 PM, Wednesday, December 3. The report should follow the department's design-report guidelines. Data should be in the form of graphs and tables, since this both condenses the results and makes them easily understandable. The appendix should include your spreadsheet and a hand calculation for at least one representative case. Hand calculations should be made using a pencil.

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.

Short-term Group Assignments

<u>Due Monday, November 10</u>

Solve the material balance for the case where $T = 450°C$; $P = 100$ atm; Purge-to-recycle ratio = 1/20. Note that the hydrogen-to-nitrogen ratio = 3.000 in every stream. Use $N_3 = 100$ kmol/h as the basis for your calculation.

<u>Due Monday, November 17</u>

Set up an Excel spreadsheet to calculate the material balance where T, P and purge-to-recycle ratio are entered manually. Scale the spreadsheet to produce 50,000 tonne NH_3/year. Run two cases for 1) $T = 450°C$; $P = 100$ atm; Purge-to-recycle ratio = 1/20 and 2) $T = 420°C$; $P = 50$ atm; Purge-to-recycle ratio = 1/10.

Due Wednesday, November 19

Expand Excel spreadsheet to include operating costs so that an annual profit or loss can be calculated for any set of operating conditions. Run two cases for 1) T = 450°C; P = 100 atm; Purge-to-recycle ratio = 1/20 and 2) T = 420°C; P = 50 atm; Purge-to-recycle ratio = 1/10.

Supplemental Information

Value of Feeds and Products

Hydrogen fresh feed	\$0.72 per pound
Nitrogen fresh feed	\$0.02 per pound
Methane in feed or purge	\$0.18 per pound
Hydrogen in purge	\$0.45 per pound
Ammonia product	\$0.30 per pound

Variable Operating Costs

Cooling after reactor	\$0.005 per lb of gas in Stream 4
Compressors	\$0.004(ΔP) per kg-mol

When calculating ΔP, assume that the fresh feed is supplied at 10 atm, and assume that Stream 9 before the recycle compressor is at 8 atm.

Fixed Operating Costs

Operating the ethanol production unit involves additional costs such as labor, maintenance and debt service which should remain nearly constant as operating parameters change. Assume that these fixed costs are \$0.05 per kg of ammonia produced.

Profit (Loss) on Unit

At a selling price of \$0.30 per pound, the value of 50-million kg of ammonia is \$33.0 million. In estimating profit or loss for various operating conditions, the significant figure for profit should be \$0.1 million.