Laboratory and Homework Assignment 9

Reading Assignment

1. "Chapter 5: Mass Balances with Recycle Streams" from Finlayson, Bruce A. Introduction to chemical engineering computing. John Wiley & Sons, 2012.
2. "Chapter 7: Process Simulation" from Finlayson, Bruce A. Introduction to chemical engineering computing. John Wiley & Sons, 2012.

Laboratory Assignment (Due after laboratory session)

1. In this exercise we will understand convergence algorithms using ammonia manufacture process as shown in Figure 1. The process takes hydrogen and nitrogen (in a 3:1 ratio) to make ammonia. The flow rates of nitrogen and hydrogen into the process are 100 and 300 mol per unit time, respectively, but there is also 1 mole per unit time of carbon dioxide. The reactor is limited by equilibrium and 25 mol% of N_2 is converted per pass. A purge stream is added to the recycle stream to stop accumulation of carbon dioxide in the process. The purge stream is 1 mol% of the recycle stream. This exercise needs to be done in Matlab and ASPEN. Use Lee-Kister-Plocker equation of state for computing thermodynamic equilibrium properties in ASPEN.

   (a) [50 points] Tear stream 7 and compute converged composition and flow rates of each stream using method of successive substitution. Do you achieve convergence, if yes in how many steps. If no, why?

   (b) [50 points] Tear stream 2 and compute converged composition and flow rates of each stream using Wegstein's method. Comment on the convergence of this method.

   The K-values for flash separation are: nitrogen, 4.8; hydrogen, 70; ammonia 0.051; carbon dioxide, 0.32. The equilibrium equation for the reactor is given by:

$$N_2 + 3H_2 \leftrightarrows NH_3 \tag{1}$$

   [Hint:] You need to solve Rachford-Rice equations for the flash separation.

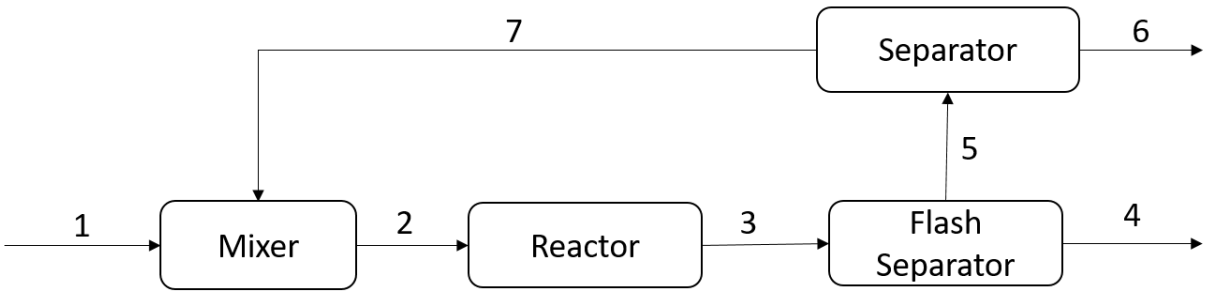

Figure 1: Ammonia manufacture process.

Practice Homework Assignment

1. [50 points] Ethyl chloride is manufactured in an integrated process; see Figure 2. Ethane reacts with chlorine to make ethyl chloride and hydrogen chloride, and ethylene reacts with hydrogen chloride to form ethyl chloride.

$$C_2H_6 + Cl_2 \leftrightarrows C_2H_5Cl + HCl \tag{2}$$
$$C_2H_4 + HCl \leftrightarrows C_2H_5Cl \tag{3}$$

The process is fed with two streams: Chlorine (1) and ethane/ethylene (2). The ethane and ethylene have the same molar flow rate, and the ratio of chlorine to ethane plus ethylene is 1.5. The ethane/ethylene stream also contains 1.5 percent carbon dioxide. The feed streams are mixed with an ethylene recycle stream and go to the first reactor (chlorination reactor) where ethane reacts with chlorine with a 95% conversion per pass. The product stream (4) is cooled and ethyl chloride is condensed and separated. Assume that all the ethane and ethyl chloride go out in the condensate stream. The gases go to another reactor (hydro-chlorination reactor) where the reaction with ethylene takes place with a 50 % conversion per pass. The product stream (7) is cooled to condense ethyl chloride, and the gases (predominately ethylene and chlorine) are recycled. A purge or bleed stream (11) takes off a fraction of the recycle stream (use 1 percent). You need to do this exercise in Matlab. Do you require to tear a stream for sequential modular approach. If yes, what are the options to tear the stream? Determine the most efficient tear stream using both successive substitution and Wegstein's method. Now perform this exercise in ASPEN. The analysis should be presented in a word file. To get any points for this problem, you should elaborate step-by-step procedure with proper justifications of your calculations.

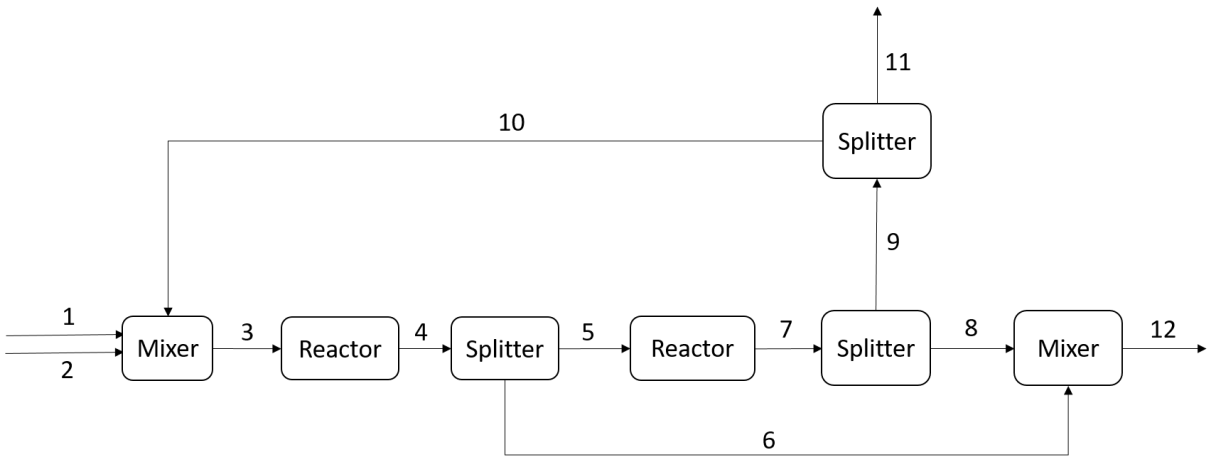

Figure 1: Ethyl chloride manufacture process.