Recycle and Purge in the Synthesis of Methanol

Methanol (also known as methyl alcohol and wood alcohol) is used as a raw material in the manufacture of formaldehyde, acetic acid, methyl tertiary-butyl ether (MTBE), and a number of other important chemicals. It also has many other uses, including as a solvent, a disinfectant, and a clean-burning fuel. One of the ways it can be synthesized is by reacting carbon dioxide and hydrogen:

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$$

The fresh feed to a methanol synthesis process contains hydrogen, carbon dioxide, and 0.400 mole% inerts (I). The reactor effluent passes to a condenser that removes essentially all of the methanol and water formed and none of the reactants or inerts. The latter substances are recycled to the reactor. To avoid buildup of the inerts in the system, a purge stream is withdrawn from the recycle.

The feed to the *reactor* (not the fresh feed to the process) contains 28.0 mole% CO_2, 70.0 mole% H_2, and 2.00 mole% inerts. The single-pass conversion of hydrogen is 60.0%. Calculate the molar flow rates and molar compositions of the fresh feed, the total feed to the reactor, the recycle stream, and the purge stream for a methanol production rate of 155 kmol CH_3OH/h.

(a) Choose a basis of calculation of 100 mol of the feed to the reactor (a convenient basis since you know the composition of this stream), and draw and label a flowchart.

(b) Perform a degree-of-freedom analysis for the system. As a suggested sequence, determine the difference between the number of equations and number of variables for each of the following: overall system, recycle-fresh feed mixing point, reactor, condenser, and recycle-purge splitting point. Verify that there are zero degrees of freedom for the entire process and identify an efficient procedure for carrying out the calculations (including scaling up the calculated process variables to the desired methanol production rate).

(c) Write the system equations and use Excel's Solver to solve them for all of the variables.

(a) Basis: 100 mol Combined Feed to the Reactor