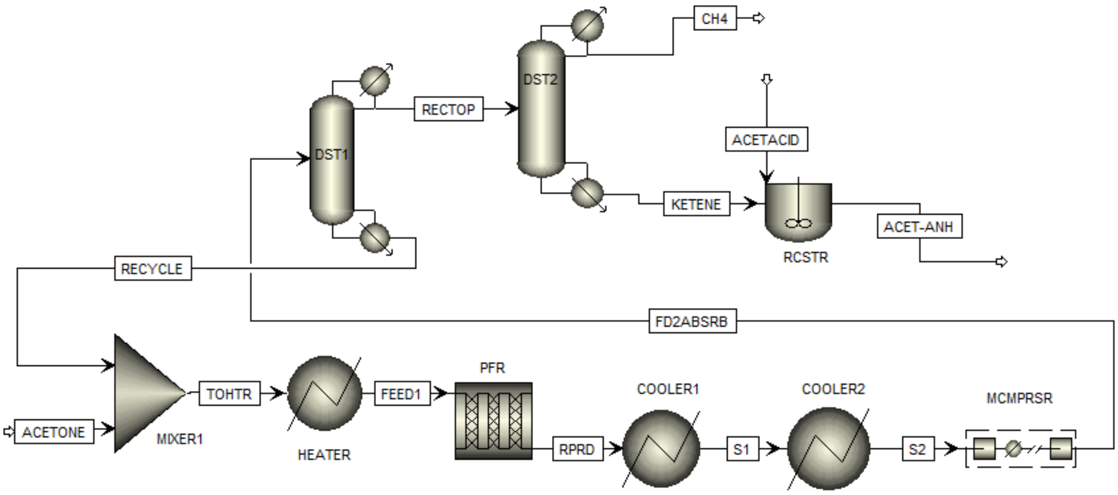
Production of Acetic Anhydride



Component list: ACETONE (CH3COCH3), KETENE (C2H2O), METHANE (CH4), ACETIC-ACID (CH3COOH), and ACETIC-ANHYDRIDE (ACET-ANH)

The methods recommended by Aspen for Carboxylic Acids are activity coefficient methods with Nothangel or Hayden-O'Connel model with vapor phase association with NRTL-HOC or WILSON-NTH.In this simulation Wilson-NTH is chosen.

All the missing binary interaction coefficients can be estimated by on UNIFAC method which use information about the structure of particular components to predict its behaviour.

The mixer and heater unit operation units haven been discussed during the previous practical session.

The reactor design in Aspen Plus depend on the reactor type the user choose. In this exercise the PFR and CSTR reactor are used. First reactor is PFR. Firstly, one needs to decide about the reactor type. The adiabatic reactor is use in this case. Then the reactor dimensions should be provided. The third step is to define the kinetics of the reaction need to be define. The powerlow model is used. Kinetic data can be found in "Elements of Chemical Reaction Engineering", Example 12–2 Production of Acetic Anhydride, written by H. Scott Fogler.

Due to the fact that outlet stream from the reactor contains high amount of unreacted acetone, which should be separated and recirculated. This can be done with absorption column or distillation column.

Although, the vapor feed to the column should be compressed before the separation. The 4-stage compressor can be used for that purpose.

Then the stream is fed into column. This is example of rare process which belong to the cryogenic group due to the very lower temperature in condenser. The acetone is bottom product and is recycled. In the second column the methane is separate from ketene in distillation column.

The ketene is a bottom product of the distillation and is used as a feed for the CSTR reactor. The ketene is mixed with acetic acid in the reactor. The information about working conditions (T and P) and technical details of reactor (Volume) are needs to be introduce to Aspen Plus. Then the reaction is described. The powerlaw model is used once again, but this time the reaction type is "equilibrium", which means that the Gibbs energy minimization algorithm is used.

All details can be found in Aspen plus: Chemical Engineering Applications / Dr. Kamal I.M. Al-Malah.

A portion of the Aspen Plus-generated “Input File” pertaining to process:

COMPONENTS: CH3COCH3/C2H2O/CH4/CH3COOH/ACET-ANH/WATER.

PROPERTIES: WILS-NTH, TRUE-COMPS=YES, ESTIMATE ALL.

STREAM ACETACID: TEMP=25◦C, PRES=15 bar, MOLE-FLOW CH3COOH 17.126 kmol/hr.

STREAM ACETONE: TEMP=25◦C. PRES=1.6 <atm> MASS-FLOW=1000 kg/hr of pure CH3COCH

BLOCK MIXER1 MIXER: PARAM

BLOCK COOLER1 HEATER: Outlet TEMP=140◦C. PRES=0 (i.e., ΔP=0). UTILITY-ID=GLPSTEAM.

BLOCK COOLER2 HEATER: PARAM TEMP=90◦C. PRES=0 (i.e., ΔP=0). UTILITY-ID=AIR

BLOCK HEATER HEATER: PARAM TEMP=1035 K, PRES=1.6 <atm>, MAXIT=40. UTILITY-ID=FH1000.

BLOCK DST1 RADFRAC: PARAM NSTAGE=14, ALGORITHM=STANDARD MAXOL=25, DAMPING=NONE, COL-CONFIG CONDENSER=TOTAL, REBOILER=KETTLE, FEEDS FD2ABSRB #7 ABOVE-STAGE, PRODUCTS: RECYCLE #14 Liquid / RECTOP #1 Liquid, P-SPEC: Stage #1 @ 29 bar, COL-SPECS: Bottom/Feed Ratio=1.0, MOLE-RR=6. Bottom/Feed PARAMS: Feed Stream=FD2ABSRB Component Basis=CH3COCH3. COND-UTIL=REFRIG4, and REB-UTIL=HPSTEAM.

BLOCK DST2 RADFRAC: PARAM NSTAGE=14 ALGORITHM=STANDARD MAXOL=75 LL-METH=HYBRID & DAMPING=MEDIUM, PARAM2 SALTS=IGNORE-CHECK, COL-CONFIG CONDENSER=TOTAL, REBOILER=KETTLE, FEEDS RECTOP #7 ABOVE-STAGE, PRODUCTS: KETENE #14 Liquid / CH4 #1 Liquid, P-SPEC: Stage #1 @ 28 bar, COL-SPECS: Distillate/Feed=0.9999, MOLE-RR=4, Distillate/ Feed PARAMS: Feed Stream=RECTOP Component Basis =CH4. COND-UTIL=REFRIG4 and REB-UTIL=LPSTEAM

BLOCK RCSTR RCSTR: PARAM TEMP=75◦C. PRES=15 bar. NPHASE=1 PHASE=L, RES TIME=1.5 <hr> BLOCK-OPTION FREE-WATER=NO REACTIONS RXN-IDS=R-2. UTILITY UTILITY-ID=CWATER.

BLOCK PFR RPLUG: PARAM TYPE=ADIABATIC LENGTH=3. <meter> DIAM=1. <meter> & PRES=1.6 <atm> REACTIONS RXN-IDS=R-1.

BLOCK MCMPRSR COMPR: PARAM NSTAGE=4 TYPE=ASME-ISENTROPIC PRES=29 bar. COOLER-NPHAS=1 & SB-MAXIT=30 SB-TOL=0.0001, FEEDS: S2 at stage #1, PRODUCTS: FD2ABSRB at stage #4, COOLER-SPECS: #1 DUTY=0 / #2 TEMP=150◦C / #3 TEMP=150 ◦ C / #4 DUTY=0, BLOCK-OPTION FREE-WATER=NO, COOLER-UTL=AIR, and SPECS-UTL=ELECTRIC.

REACTIONS R-1: POWERLAW, REAC-DATA 1 PHASE=V, RATE-CON 1 PRE-EXP= 8.19733E+014 ACT-ENERGY=284521.7 <kJ/kmol> STOIC 1 MIXED CH3COCH3 -1. / C2H2O 1. / CH4 1. POWLAW-EXP 1 MIXED CH3COCH3 1.

REACTIONS R-2: POWERLAW, REAC-DATA 1 EQUIL, STOIC 1 MIXED C2H2O -1. / CH3COOH -1. / ACET-ANH 1.

Aspen Process Economic Analyzer

The costing options include the selection of the basis for cost estimation, defining feed and product stream prices, and defining utilities in terms of pricing and associating them with pieces of equipment, such as a pump, compressor, condenser, reboiler, and heater.

1. Information about operating life plant, length of plant start-up and start of basic engineering.

2. Feed and Product Stream Prices.
   They are not required for the estimation of equipment cost, but if one want to make full economic analysis all raw materials and product prices should be described. The values have been added into simulation in advance.

3. Utility Association with a Flowsheet Block
   They are not required for the estimation of equipment cost, but if one want to make full economic analysis all raw materials and product prices should be described. The values have been added into simulation in advance.

4. Economic analysis can be handled in Aspen Plus or APEA software.

5. Mapping.
   Each peace of equipment needs to be mapped, which means that the type of equipment should be specified. In our case:

   a. COOLER1 is "Floating head shell and tube exchanger" because of significant temperature difference between the hot and cold stream.
   b. COOLER2 is "TEMA Shell-and-Tube"
   c. "DST1(RADFRAC)" and "DST2(RADFRAC)".
      The distillation columns consist the sets of equipment, and each of the should be specify.
      Tower type is "Multiple diameter, trayed or packed tower".
      Condenser type is "Bare pipe immersion coil".
      Condenser drum is "Horizontal drum"
      Reflux pump type is "Centrifugal single or multi-stage pump".
   d. Heater type is "Box type process furnace".
   e. Mixer can be represented as "Agitated tank – enclosed".
   f. The compressor type is "Centrifugal compressor - horizontal".
   g. PFR is "Packed tower".
   h. CSTR is "Agitated tank – enclosed, jacketed".

6. Fixing Geometrical Design-Related Errors
   At this point all errors corelated to the size of equipment should be spotted and fixed. The second type of error which should be consider is the selection/modification of material of construction. In our example:
   a. HEATER require to modify the material modification. The default Carbon steel A214 can be replaced with S347.
   b. COOLER1 material can be specified as "347S" and "SS347" for construction for both tube and shell.
   c. The packing in PFR is "1.0 CRR Ceramic raschig ring".
   d. Feel free to get crazy and change other materials on your own.

7. The final evaluation of the project