Process Simulation with ASPEN Plus

7505 Course Notes

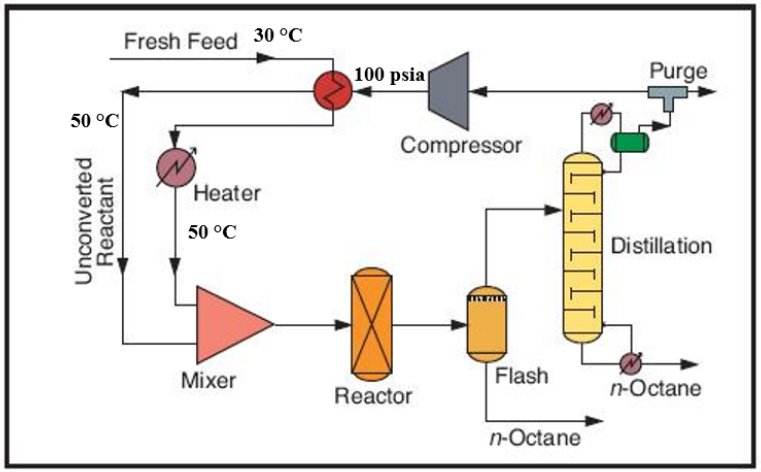
Section 7: Putting It All Together:

Simulating Complex Chemical Processes

These course materials are applicable to Version 14 of ASPEN Plus

Chemical Process #1

- **n**-Octane Production Process



Problem Statement with Input Data

The compound *n*-octane can be produced from ethylene (C_2H_4) and *i*-butane (C_4H_{10}) in an adiabatic stoichiometric reactor (ΔP = 2 psia) according to the reaction:

$$2C_2H_4 + i\text{-}C_4H_{10} \rightarrow C_8H_{18}$$

Temperatures and pressures are given for some of the streams. Notice that this process produces two grades of *n*-octane, namely low-grade and high-grade octane. The low-grade is recovered as the bottom of the flash which has a lower purity ($\geq$ 95 mol%) than the high-grade ($\geq$ 99 mol%) produced from the bottom of the distillation column.

Problem Statement with Input Data (Cont'd)

The fresh feed contains in kmol/hr 1.0 nitrogen (N_2), 100 ethylene (C_2H_4), 3.0 *n*-butane (n-C_4H_{10}), and 50 *i*-butane (i-C_4H_{10}) at 30°C and 20 psia.

The following data are also known about the process:

1. The flash vessel is isobaric (i.e. inlet and outlet pressures are equal or $\Delta P = 0$ with cooling to condense enough *n*-octane.)
2. The pressure drops across the heat exchanger, the heater, and the mixer are considered negligible.
3. The compressor is isentropic, and the purge takes out 5% of the column overhead.

Problem Statement with Input Data (Cont'd)

4. The column (short-cut model) operates at 3.0 times the minimum reflux ratio and recovers 99.50 mol% *n*-butane in the overhead and 99.90 mol% *n*-octane in the bottom.

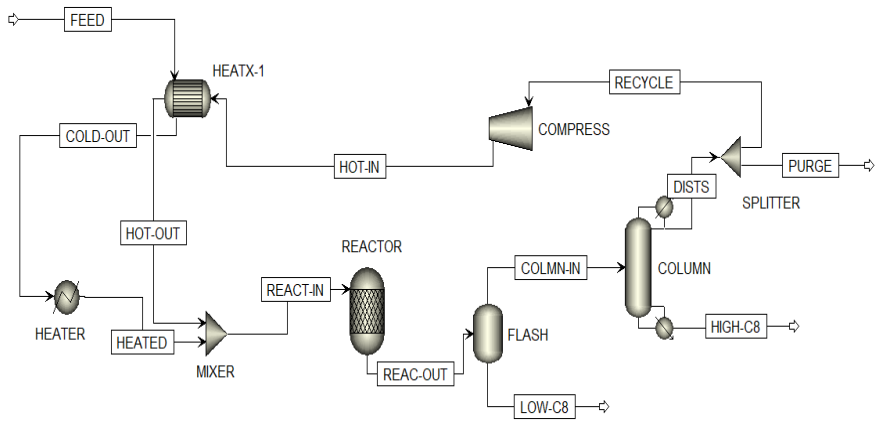
5. The condenser of the column is partial with all vapor distillate and its pressure is 15 psia. The pressure in the reboiler is 16 psia.

6. The process must produce 20 kmol/hr of low-grade *n*-octane from the flash vessel.

7. The conversion of the reaction is 90 mole% based on ethylene.

Use ASPEN Plus to simulate this *n*-octane production process. For properties, use the Peng-Robinson equation of state.

Process Flow Diagram from A+ for Process #1



Important Stream Results for Process #1

Material | Heat | Load | Work | Power | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	LOW-C8	HIGH-C8
+ Mole Flows	**kmol/hr**	**20**	**30.8988**
− Mole Fractions			
N2		0.000841952	5.32341e-08
ETHYLENE		0.00145436	1.83353e-06
I-BUTANE		0.00347028	0.000665335
N-BUTANE		0.0429402	0.0063301
N-OCTANE		0.951293	0.993003
+ Mass Flows	**kg/hr**	**2228.58**	**3517.47**
+ Mass Fractions			

One Design-Spec in Process #1

Flash vapor fraction

Main Flowsheet | REACTOR (RStoic) | Control Panel | Convergence | **DS-1 - Results**

Results | Status

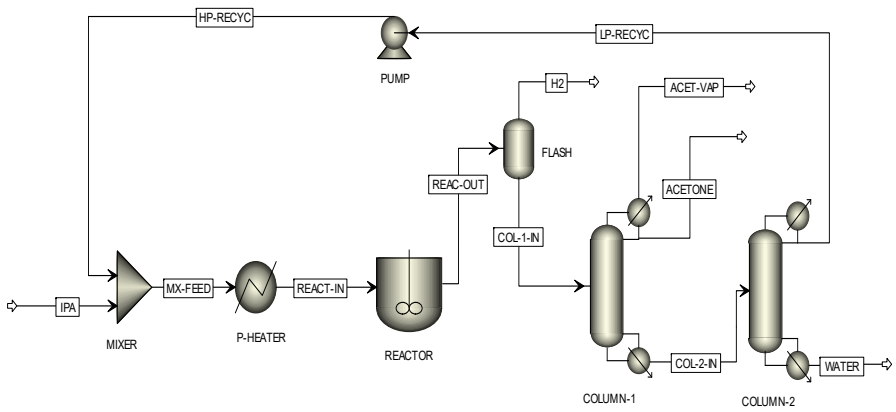
Variable	Initial value	Final value	Units
MANIPULATED	0.839096	0.839376	
C8FLOW	20.0348	20	KMOL/HR

Summary | Balance | Phase Equilibrium | Utility Usage | Status

Outlet temperature	92.8463	C
Outlet pressure	18	psia
Fluid phase vapor fraction (Mole)	0.839376	
Fluid phase vapor fraction (Mass)	0.755206	
Heat duty	-2.11685	Gcal/hr
Net duty	-2.11685	Gcal/hr
1st liquid / Total liquid	1	
Pressure drop	0	psia

Chemical Process #2

- Acetone Production Process



Problem Statement with Input Data

A process to produce acetone by dehydrogenation of isopropyl alcohol (IPA) is to be simulated using ASPEN Plus. Fresh IPA with a small amount of water is fed to a preheater and then to a continuous stirred tank reactor in which the following endodermic reaction occurs:

$$(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$$

A flash vessel is used to purge the hydrogen product from the reactor effluent, while the liquid goes into a distillation column which separates out acetone as a product in the overhead. A second distillation column is required to separate water from unreacted IPA so that the alcohol can be recycled back to the reactor via a high-pressure pump.

Problem Statement with Input Data (Cont'd)

The following data and operating conditions are available:

Feed stream:	
Composition (mole fractions)	
IPA	0.85
Water	0.15
Total Flow (lbmol/hr)	500.0
Temperature (°F)	100.0
Pressure (psia)	30.0
Recycle Pump:	
Outlet pressure (psia)	30.0
Feed Preheater:	
Outlet temperature (°F)	550.0
Pressure drop (psi)	3.0

Problem Statement with Input Data (Cont'd)

Reactor:

Reactor type	Adiabatic CSTR
Reaction (gas phase)	$(CH_3)_2CHOH \rightarrow (CH_3)_2CO + H_2$
Reactor volume (ft^3)	2500
Phase calculations	Vapor-liquid (because the reaction is endothermic and may result in some condensation)
Kinetics: 1st-order power-law reaction	$r_{IPA} = 5.25\times10^5 e^{-15000/RT}[(CH_3)_2 CHOH]$ where E is in the unit of Btu/lbmol.
Pressure drop (psi), DP	Based on the following empirical correlation $DP = \frac{2.85\times10^6 \phi^{3/2} x_{ACETONE}^2}{T}$

Stream REAC-IN { where ϕ = mass-density (lbm/ft^3), $x_{ACETONE}$ = mole fraction of acetone, T = temperature

Problem Statement with Input Data (Cont'd)

Flash:

Heat loss	Negligible
Pressure drop	Negligible

Column-1 (rigorous model):

Number of stages	50
Feed tray location	25
Reflux ratio (molar basis)	3.0
Distillate to feed ratio (mole basis)	0.60
Pressure in condenser (psia)	15.0
Pressure in reboiler (psia)	16.0
Condenser	Partial with both vapor and liquid distillates
Design target	Loss of acetone from the column as vapor distillate is limited to exactly 10 lbmol/hr.

Problem Statement with Input Data (Cont'd)

Column-2 (rigorous model):

Number of stages	30
Feed tray location	15
Reflux ratio (molar basis)	3.0
Pressure in condenser (psia)	12.0
Pressure in reboiler (psia)	13.0
Condenser	Total
Design target	Concentration of IPA in the wastewater stream (Stream WATER) must be limited to 1.0 mole%

Use NRTL-RK as the property method in your simulation while declaring hydrogen as Henry's Law component. The reason why NRTL-RK must be used is that IPA, water, and acetone form a highly nonideal solution. In fact, IPA and water form an azeotrope at 31.7 mol% IPA, but luckily the water concentration in Stream COL-2-IN with lots of acetone is higher than this number so we are able to separate water to very high purity.

Problem Statement with Input Data (Cont'd)

Notes: To converge this flowsheet and obtain a correct solution, correct property parameters must be used. Be sure to visit Methods → Parameters →Binary Interaction → NRTL-1 menu and see that 3 pairs of binary interaction parameters are retrieved from APV140 VLE-IG Databank. More importantly, make sure that you visit HENRY-1 menu too and select all 3 databanks (APV140 BINARY, APV140 ENRTL-RK APV140 HENRY-AP) in the Databanks sheet so that Henry's Law constants between H_2-water and H_2-acetone are retrieved as well.

Answer the following questions:

1. ΔP across the reactor = 1.74 psia

2. % conversion of the reaction based on IPA = 95.56 %

3. Temperature of the condenser in Column-1 = 133.69 °F

4. Product purity (mole%) of acetone in liquid distillate of Column-1 = 97.10 %

Important Stream Results for Process #2

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	ACET-VAP	ACETONE
WATER	lbmol/hr	0.270521	4.36061
H2	lbmol/hr	0.096334	0.00055666
IPA	lbmol/hr	0.000243301	0.00592749
ACETONE	lbmol/hr	10	145.999
− Mole Fractions	From design-spec		
WATER	in Column 1	0.0260942	0.0289999
H2		0.00929229	3.70203e-06
IPA		2.34686e-05	3.94203e-05
ACETONE		0.96459	0.970957

Important Stream Results for Process #2

	Units	LP-RECYC	WATER
Average MW		54.2774	18.4361
+ Mole Flows	**lbmol/hr**	**64.7805**	**42.375**
− Mole Fractions			
WATER		0.104027	0.99
H2		0	0
IPA		0.181167	0.01
ACETONE		0.714806	3.72055e-12
+ Mass Flows	**lb/hr**	**3516.12**	**781.23**

From design-spec in Column 2

Calculator Block Result for Process #2

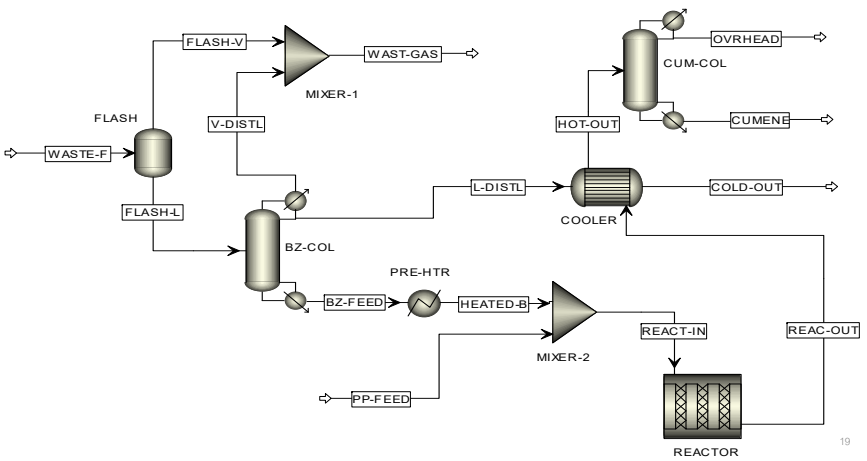
Main Flowsheet | Control Panel | C-1 - Results | **REACTOR (RCSTR) - Stream Results (Boundary)**

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	REACT-IN	REAC-OUT
Stream Class		CONVEN	CONVEN
Maximum Relative Error			9.64732e-05
Cost Flow	$/hr		
− MIXED Substream			
Phase		Vapor Phase	
Temperature	F	550	119.496
Pressure	psia	27	25.2635
Molar Vapor Fraction		1	0.727177
Molar Liquid Fraction		0	0.272823

Chemical Process #3

- Cumene Production Process (Highly Constrained)



Problem Statement with Input Data

A wastewater stream with 50 mol% benzene is to be treated to remove impurities so it could be used to produce cumene (isopropyl benzene). The wastewater first enters a flash to remove light gases. The liquid from the flash then enters a distillation column to separate out high-purity benzene in the bottom stream. After that, this liquid benzene is pre-heated to a super-heated state and combined with propylene (100% pure at 200 °F and 14.7 psia). Benzene and propylene are then allowed to react to form cumene in an isothermal plug flow reactor. The reactor effluent is cooled in a heat exchanger by the liquid distillate from the first column. A second distillation column is used to purify cumene which exits as the bottom product. The cumene reaction is as follows:

$$\underset{\text{propylene}}{C_3H_6} + \underset{\text{benzene}}{C_6H_6} \rightarrow \underset{\text{cumene}}{C_9H_{12}} \qquad \text{(gas phase reaction)}$$

Problem Statement with Input Data (Cont'd)

The following additional data are known about the process:

1. The temperature of the wastewater feed is 100 °F and its pressure is 20 psia. Its composition is: 15% acetone, 50% benzene, 15% methanol, 10% methane, 6% acetylene (C_2H_2), 3% nitrogen, and 1% oxygen (all molar basis), and the total flow rate is 200 lbmol/hr.
2. The wastewater stream is flashed at 0 °F with negligible pressure drop.
3. The first column (BZ-COL) has 20 theoretical stages, which include a partial condenser ($P_{condenser}$ = 14 psia) and a reboiler ($P_{reboiler}$ = 15 psia). The feed tray location is 15. The column operates with a molar reflux ratio of 3 and takes out 90 lbmol/hr in the bottom stream.
4. The pre-heater vaporizes the benzene stream and superheats it to 30 °F above its dew-point temperature. The pressure drop inside the pre-heater is 0.3 psia.
5. The waste gas stream (WAST-GAS) has a total flow rate of 37.0 lbmol/hr.
6. The plug flow reactor has a diameter of 1.2 ft with negligible pressure drop. The kinetics for the cumene reaction follows the power-law expression and is given as:

Problem Statement with Input Data (Cont'd)

$$r_{propylene} = kC_{propylene}C_{benzene}$$

$$k = 1.5\times10^{4}\exp\left(\frac{-5500}{RT}\right)$$

where the unit of the activation energy is Btu/lbmol and C_i is molar concentration. The conversion of the cumene reaction is maintained at 99%.

7. The plug flow reactor is operated isothermally at the same temperature as that of the inlet to the reactor (REAC-IN). Note that although the cumene reaction occurs in the gas phase, you must specify Valid Phases = Vapor-Liquid in RPLUG because the generation of cumene may cause liquid to form inside the reactor.
8. The exit temperature of the cold side in the cooler is 100 °F. This cooler has negligible pressure drop.

Problem Statement with Input Data (Cont'd)

9. The cumene column (CUM-COL) consists of 10 theoretical stages, which include a total condenser ($P_{condenser}$ = 14 psia) and a reboiler ($P_{reboiler}$ = 14.5 psia). The feed tray location is 5. The column takes out 20 mol% of the feed as the overhead distillate and operates with a molar reflux ratio of 3.
10. The cumene product stream from the second column must contain a purity of 99.5 mole% cumene (product spec).

Answer the following questions:

1. Temperature of the condenser in BZ-COL = 6.92 °F

2. Molar ratio of propylene to benzene in the reactor inlet (REAC-IN) = 1.194

3. Reactor length = 11.93 feet

Important Stream Results for Process #3

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	CUMENE
ACETONE		3.6668e-07
BENZENE		0.00499962
METHANOL		2.1539e-08
CH4		4.83842e-28
C2H2		5.72433e-21
N2		0
O2		0
PROPYLEN		3.25845e-09
CUMENE		0.995

Important Design-Spec Results for Process #3

Variable	Initial value	Final value	Units
MANIPULATED	11.9311	11.9311	FT
BZOUT	0.872467	0.872467	LBMOL/HR
BZIN	86.5936	86.5936	LBMOL/HR

	Units	REACT-IN	REAC-OUT
− Mole Flows	**lbmol/hr**	**193.411**	**107.69**
ACETONE	lbmol/hr	3.39934	3.39934
BENZENE	lbmol/hr	86.5936	0.872467
METHANOL	lbmol/hr	0.00709585	0.00709585
CH4	lbmol/hr	7.49165e-12	7.49165e-12
C2H2	lbmol/hr	2.42446e-09	2.42446e-09
N2	lbmol/hr	1.38729e-22	1.38729e-22
O2	lbmol/hr	2.36463e-21	2.36463e-21
PROPYLEN	lbmol/hr	103.411	17.6897

Important Design-Spec Results for Process #3

Variable	Initial value	Final value	Units
MANIPULATED	100	103.411	LBMOL/HR
XCUMENE	0.999992	0.995	

	Units	CUMENE
METHANOL		2.1539e-08
CH4		4.83842e-28
C2H2		5.72433e-21
N2		0
O2		0
PROPYLEN		3.25845e-09
CUMENE		0.995
+ Mass Flows	**lb/hr**	**10336.8**

Important Design-Spec Results for Process #3

Variable	Initial value	Final value	Units
MANIPULATED	0.05	0.0470778	
WASTEGAS	37.2239	37	LBMOL/HR

	Units	WAST-GAS
Average MW		22.0276
− Mole Flows	**lbmol/hr**	**37**
ACETONE	lbmol/hr	0.277271
BENZENE	lbmol/hr	0.185697
METHANOL	lbmol/hr	0.0711465
CH4	lbmol/hr	19.1228
C2H2	lbmol/hr	9.34333
N2	lbmol/hr	5.99987
O2	lbmol/hr	1.99984