Process Simulation of Alkylation of 1-Butene to Octane and Dodecane

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A. Background

N-Octane is an alkane with the molecular formula C_8H_{18}. Octane is a component of gasoline (petrol). Octane is volatile and very flammable. N-Octane exists as liquid at room temperature with a boiling point of 125°C and a melting point of -57°C. N-Octane is insoluble in water [1].

N-Dodecane is also known as Dihexyl, Bihexyl, Adakane 12 or Duodecane. N-Dodecane is a liquid alkane hydrocarbon. It is an oily liquid of the paraffin series. N-Dodecane is used as solvent, distillation chaser and also as a scintillator component [2].

B. Description of Flow Sheet

This flow sheet was adapted from Luyben (2009) [3].

The feed containing 67 mole percent of 1-Butene and 33 mole percent of Hydrogen was first pre-heated to a temperature of 475°C and then fed to an equilibrium reactor where reaction takes place at 3 bar pressure. The product stream from the reactor, containing N-Octane and unreacted 1-Butene and Hydrogen was cooled to 10°C at constant pressure and was fed to a gas-liquid separator. In the gas-liquid separator most of the Hydrogen present in the product stream was removed as vapor and the remaining product stream was obtained as liquid. The liquid stream was then split into two separate streams having equal mass flow rates. One stream was heated to 300°C at 3 bar pressure and was fed to another equilibrium reactor where N-Dodecane was obtained as product. The product stream also contains unreacted N-Octane and 1-Butene. The products were sent into a shortcut column where 1-Butene was obtained as distillate and N-Octane and N-Dodecane as bottom stream. The bottom stream was then sent to another shortcut column where N-Octane was obtained as the distillate stream and N-Dodecane as bottoms. The second stream from the

splitter was fed to another shortcut column where N-Octane was obtained as the bottom product and 1-Butene as distillate. All the products were then cooled to room temperature.

C. Results

The process flow sheet for the Alkylation of 1-Butene to N-Octane and N-Dodecane was simulated at a temperature of 475°C and 300°C respectively. Three shortcut distillation columns were simulated to calculate the actual number of stages, minimum number of stages, location of feed stage and minimum reflux ratio for the given light key and heavy key compositions. In the first shortcut distillation column, 1-Butene was taken as the light key component and N-Dodecane was taken as the heavy key component. The light key composition at the bottoms was fixed at 0.01 and the heavy key composition in the distillate was fixed at 0.001 and a reflux ratio of 10 was assumed for the first shortcut column. The shortcut column was simulated and a minimum reflux ratio of 8.17 was obtained with actual number of stages equal to 3. In the second shortcut distillation column, N-Octane was taken as the light key component and N-Dodecane was taken as the heavy key. The light key composition at the bottoms was fixed at 0.001 and the heavy key composition in the distillate was fixed at 0.001. A reflux ratio of 3 was assumed for the shortcut column. The shortcut column was simulated and a minimum reflux ratio of 0.02 was obtained with actual number of stages equal to 4. In the last shortcut distillation column, 1-Butene was taken as the light key component and N-Octane as the heavy key component. The light key composition at the bottoms was fixed at 0.0001 and the heavy key composition in the distillate was fixed at 0.001 and a reflux ratio of 5 was assumed for this shortcut column. The shortcut column was simulated and a minimum reflux ratio of 0.01 was obtained with actual number of stages equal to 4. The results obtained from the three shortcut distillation columns were used to specify the input parameters for the simulation of three rigorous distillation columns respectively. The first rigorous column was operated at a condenser pressure of 2 bar and reboiler pressure of 1.01325 bar. The product molar flow rate was assumed to be 6.7177 kmol/h and a reflux ratio of 10 was assumed. Similarly the second rigorous distillation column was operated at a condenser pressure of 1.01325 bar and at a reboiler pressure of 0.5 bar. A reflux ratio of 3 was assumed and the product molar flow rate was taken to be equal to 1.9519 kmol/h. The third rigorous column was operated at a condenser pressure of 1.5 bar and a reboiler pressure of 1.01325 bar. The reflux ratio and

the molar flow rate of the product were assumed to be 5 and 6 kmol/h respectively. The process flow sheet for the alkylation of 1-Butene to N-Octane and N-Dodecane with three rigorous distillation columns was simulated successfully.

Results								
Object	S-1	S-15	S-16	S-19	S-20	S-23	S-24	
Temperature	25	25	50	25	25	35	25	C
Pressure	3	2	1.01325	1.01325	0.5	1.5	1.01325	bar
Mass Flow	2500	172.68137	856.52141	528.84806	327.5319	344.02723	685.1368	kg/h
Molar Flow	65.346493	3.0720654	6.7177154	4.7639896	1.9519258	5.7844491	6	kmol/h
Molar Fraction (Mixture) / 1-butene	0.67	0.99823562	0.058316609	0.081933226	1.214466E-05	0.94207302	0.00071458958	
Molar Fraction (Mixture) / Hydrogen	0.33	4.5156324E-06	2.785766E-15	3.0439228E-15	2.1096176E-21	3.451608E-06	1.3553658E-15	
Molar Fraction (Mixture) / N-octane	0	0.0017573198	0.64474315	0.89060683	0.045221673	0.057923526	0.99928541	
Molar Fraction (Mixture) / N-dodecane	0	2.5442609E-06	0.29694024	0.027459944	0.95476618	0	0	

D. Conclusion and Remarks

This study shows that open source process simulator can be used for simulating process and development of process flow sheets. This work can be extended to simulate the alkylation of 1-Butene to higher alkane hydrocarbons. Further, the unreacted components can be recycled in order to increase the productivity of the process.

Unit System: (Custom 5 in DWSIM)

Temperature - °C

Pressure - bar

Molar Flow Rate – kmol/h

Mass Flow Rate – kg/h

Volumetric Flow Rate – m3/h

Density – kg/m3

References

1. https://en.wikipedia.org/wiki/Octane

2. https://en.wikipedia.org/wiki/Dodecane

3. Luyben W.L., Design and Control of an Autorefrigerated Alkylation Process. Industrial & Engineering Chemistry Research, 2009, 48, 11081-11093