Process Flowsheet for the Production of 150 TPD 1,4-Butanediol

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A. Background

1,4-Butanediol (1,4-BDO) is a colourless, odourless viscous liquid organic compound. The IUPAC name of the compound is Butane-1,4-diol. It is mainly used as an intermediate for the production of tetrahydrofuran (THF) and polybutylene terephthalate (PBT) which are further used to produce spandex fibres, resins, solvents and printing inks, plastics and elastomers. The production capacity of 1,4-Butanediol is around 2.1 million TPA in the year 2011 and it is estimated to have a compounded annual growth rate (CAGR) of 7.1% during 2009-2030. A 1:50 scale down ratio from the global supply is taken as basis for the present work (150 TPD). BASF (Reppe process), Eastman Chemical Company (Selective epoxidation process), Misuibishi Chemical Corporation (Mitsuibishi process) and Dairen Chemical Corporation (Dairen process) are the major producers of 1,4-Butanediol all over the globe. Reppe process is chosen for process flowsheeting for the present work. This process flowsheet is developed as part of the final semester project work of the undergraduate chemical engineering degree program.

B. Description of Flow Sheet

In this process (Reppe process), acetylene is reacted with formaldehyde in the presence of copper-bismuth catalyst to produce 1,4-Butynediol which is hydrogenated to produce 1,4-Butanediol. The reactants (Acetylene and formaldehyde) are pre heated (100^{o}C) and pressurized (10 bar) and sent to the conversion reactor in which 2-Butyne-1,4-diol is formed. The exit stream of the reactor is fed into a series of distillation columns in order to separate 2-Butyne-1,4-diol in the bottom stream of the distillation column for the hydrogenation reaction. The top stream of the distillation column is further separated using a flash column and reactants are recycled back to

the reactant stream. The 2-Butyne-1,4-diol obtained from the distillation column bottom stream is mixed with hydrogen. The mixture is preheated (300^{o}C) and pressurized (350 bar) in a step-wise manner using a series of compressors and is then fed into the conversion reactor wherein the hydrogenation reaction takes place. The exit stream from the conversion reactor is fed into a distillation column in order to recover 1,4-Butandiol (product) in the bottom stream to its desired purity and quantity. The top stream of the distillation column is further separated using a flash column to recover the unreacted hydrogen and is recycled back to the reactant stream of the hydrogenation reaction. The bottom stream (product stream) from the distillation column is cooled to room temperature and sent to storage vessel.

C. Process Flow sheet

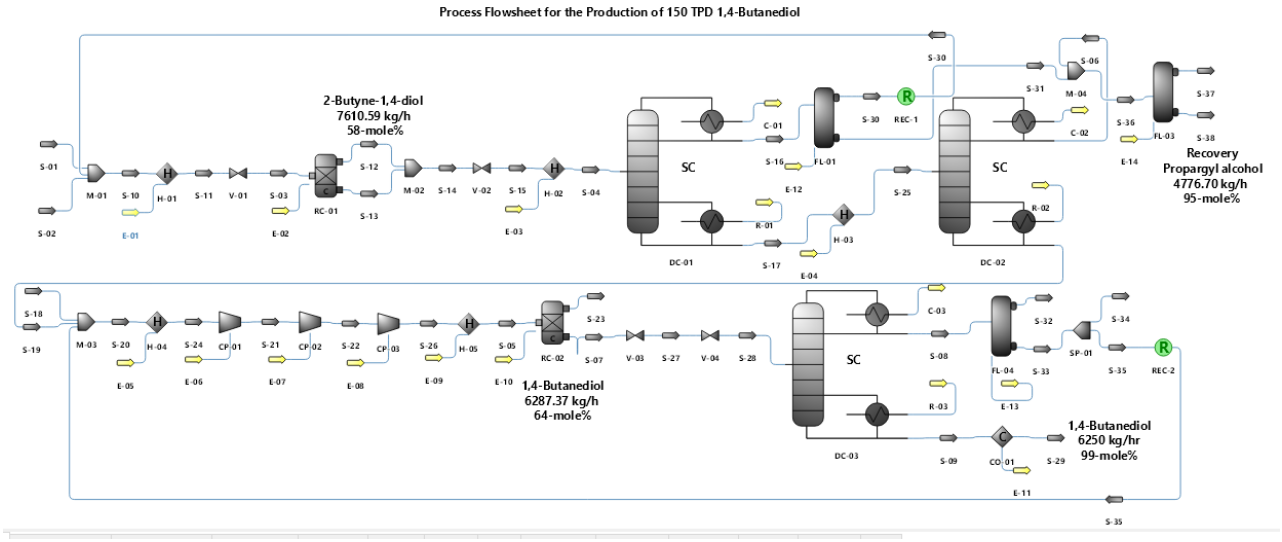

Figure 1: Process Flowsheet for the Production of 150 TPD 1,4-Butanediol (DWSIM-v-5.8)

D. Results

The process flow sheet for the production 150 TPD of 1,4-Butanediol with recycle and propargyl alcohol recovery was simulated using DWSIM (v-5.8). Peng-Robinson (PR) was chosen as the property package for simulation. Since detailed kinetic data was not available, conversion reactor with 90% conversion for the first reaction and 95% conversion for the second reaction was assumed in the simulation. A shortcut

distillation column was simulated to obtain actual number of stages and minimum reflux ratio. The operating conditions for the shortcut column were obtained through sensitivity analysis using flash column. Thus, 4776.70 kg/h (126 TPD) of 95% pure propargyl alcohol at liquid phase is recovered. 6250 kg/h (150 TPD) of 99% pure 1,4-Butanediol at liquid phase (25^{o}C and 1 bar) was obtained as the desired product.

Simulation-Results					
Object	**S-38**	**S-29**	**S-02**	**S-01**	
Temperature	45	25	25	25	**C**
Pressure	0.5	1	1	1	**bar**
Molar Flow (Mixture) / Acetylene	0.0681566	2.51672E-60	180	0	**kmol/h**
Molar Flow (Mixture) / Formaldehyde	2.83674	1.19343E-48	0	282	**kmol/h**
Molar Fraction (Mixture) / 1,4-butanediol	0	0.990002	0	0	
Molar Flow (Mixture) / 1,4-butanediol	0	69.354	0	0	**kmol/h**
Mass Flow (Mixture) / 1,4-butanediol	0	6250.25	0	0	**kg/h**
Molar Fraction (Mixture) / Propargyl Alcohol	0.951961	2.67831E-25	0	0	
Molar Flow (Mixture) / Propargyl Alcohol	85.2012	1.87628E-23	0	0	**kmol/h**
Mass Flow (Mixture) / Propargyl Alcohol	4776.7	1.05191E-21	0	0	**kg/h**

Figure 2: Simulation Results for the given process.

E. Conclusion and Recommendation

The present work demonstrates the use of open source simulation software (DWSIM) for process development and flowsheeting with ease. In the present work, conversion reactor is used for simulation. The reactor can be further designed with the help of kinetic data. The heaters and coolers in the process flow sheet can be converted into heat exchangers. The shortcut columns (B11 & B5) in the simulation show errors in two parameters – actual number of stages and optimum feed stage. These errors can be rectified and the shortcut column can be converted into rigorous distillation column.

Unit System: (UNID_9844 in DWSIM)

Molar flow rate – kmol/h

Mass flow rate – kg/h

Volumetric flow rate – m^3/h

Density – kg/m^3

Temperature - ^{o}C

Pressure – bar

Molecular weight – kg/kmol