Process Development for Production of 710 TPD of Dimethyl Carbonate by Liquid Phase Oxidative Carbonylation of Methanol

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A. Introduction:

Dimethyl carbonate is a colorless liquid with a characteristic ester-like odor, and is flammable. This compound is a green chemical with wide usage in various sectors like lithium-ion battery electrolytes and also acts as an intermediate in production of various compounds like Urea. Methods involved in the production of dimethyl carbonate are Phosgenation of methanol, ethylene carbonate transesterification, urea transesterification, direct synthesis from carbon dioxide, liquid phase synthesis of oxidative carbonylation of methanol and vapour phase methyl nitrite carbonylation. UBE Industries Ltd., Japan, EniChem, Italy are leading producers of dimethyl carbonate, producing nearly 25% of the total worldwide production. This flowsheet is developed as a part of the Chemical Engineering final semester project work.

B. Process Flow Sheet Description

Methanol, Oxygen and Carbon Monoxide which are available in 25°C and 1 bar are compressed and heated or cooled to Reactor Temperature and Pressure. SRK model was chosen for the process. Reactor is operated at 140°C and 40 bar. Conversion Reactor is used assuming a conversion of 80%. Oxygen and Carbon Monoxide are removed using Compound Separator. ChemSep Column is used to obtain 99.5% purity of dimethyl carbonate. Since higher quantity of dimethyl carbonate exist in the distillate end, a series of three distillation columns are used to obtain dimethyl carbonate of 98.25% purity. The operating temperature and pressure for each ChemSep column are obtained from sensitivity analysis performed in the Flash Column (Gas-Liquid Separator). Production of 710 TPD of dimethyl carbonate with 99% purity is achieved in stream S29. Heater, cooler, adiabatic compressor and adiabatic valve are used at appropriate streams to maintain the operating condition. Unreacted reactants that are obtained from compound separator and ChemSep column 1 are recycled back to the reactor.

C. Results:

710 TPD of Dimethyl Carbonate with 99% purity is achieved in stream S29 for the flowsheet developed. Results for important streams developed in the flowsheet are shown in Table 1.

Table 1 Results for Important Streams in Process Flow Sheet developed for Production of 710 TPD of Dimethyl Carbonate

Object	S1	S4	S7	S27	S29	S30	S31	S32	Units
Temperature	25	25	25	89.3268	25	140	68.3893	97.0186	C
Pressure	1.01325	1.01325	1.01325	1.01325	1.01325	40	1.01325	1	bar
Mass Flow	29993.7	7488.36	13109.8	9184.58	27057.6	21603.2	12063.1	17873	kg/h
Molar Flow	936.08	234.02	468.04	103.137	302.351	720	244.493	199.214	kmol/h
Molar Fraction (Mixture) / Methanol	1	0	0	0.01681	0.00573	0	0.70184	2.77E-12	
Molar Fraction (Mixture) / Oxygen	0	1	0	0	0	0.5	0	0	
Molar Fraction (Mixture) / Carbon monoxide	0	0	1	0	0	0.5	0	0	
Molar Fraction (Mixture) / Dimethyl carbonate	0	0	0	0.9825	0.99074	0	0.29807	0.995	
Molar Flow (Mixture) / Dimethyl carbonate	0	0	0	101.332	299.55	0	72.8748	198.218	kmol/h
Mass Flow (Mixture) / Dimethyl carbonate	0	0	0	9127.75	26982.9	0	6564.41	17855.1	kg/h
Molar Fraction (Mixture) / Water	0	0	0	0.00069	0.00353	0	9.19E-05	0.005	

D. Further Work:

Heaters and Coolers used in the simulation can be replaced with appropriate Heat Exchangers. Design and implementation of controllers in ChemSep Columns can be done to understand the dynamic nature of the columns.

E. References

Delledonne, Daniele & Rivetti, Franco & Romano, Ugo. (2001). Developments in the production and application of dimethylcarbonate. Applied Catalysis A: General. 221. 241-251.