Methyl Acetate Process Using Carbonylation of Dimethyl Ether Produced from Methanol

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Introduction

Methyl Acetate generally produced by esterification of the acetic acid with Methanol; but there is alternative route in which methanol is first dehydrated to Dimethyl Ether and then carbonylated to Methyl Acetate. Here, we try to simulate that alternative route. First, we develop flowsheet for Dimethyl Ether production (Figure. 1) [1] and then for Methyl Acetate (Figure. 8) [1].

(*This flowsheet development is in accordance for the FOSSEE Summer Fellowship 2019*)

Development of flowsheet in DWSIM

Thermodynamics

For Methanol-Water system in production of Dimethyl Ether, we use UNIFAC(NIST) which gives an appropriate answer for all unit operation. But for the Carbonylation route we select the Chao-Seader model because of presence of hydrogen; which gives nearly appropriate answers. Distillation column in Carbonylation, work on the DeChema-NRTL model (of ChemSep) because here, UNIFAC and Simple EOS model fail because of the presence of trash amount of hydrogen and specially water.

Description of flowsheet

Fresh feed of 500 kmol/hr containing 99 mol% Methanol and 1 mol% water is feed to the vaporizer and then passing through the cooled reactor where below reaction take place

$$2CH_3OH \Leftrightarrow CH_3OCH_3 + H_2O \quad (1)$$

Where per pass conversion of Methanol is nearly 82.88%. To utilize the heat of reactor effluent, we pass that stream through the heat exchanger which pre heat the feed of reactor coming out from the vaporizer up to 628 K. Still, effluent contain the significant amount of heat which further pass through heat economizer which increase temperature of fresh feed up to 400 K. Now, this stream (effluent coming out from the economizer) is cooled to 351 K and feed at 12th tray of 22 trays distillation column(C1) which top product is Dimethyl Ether. Bottom product of column C1 contains the mixture of Water and Methanol are feed at 16th tray of 27 trays distillation tower(C2) to remove the Water, which top product in unreacted Methanol which recycled to the Fresh Methanol Feed.

Produced Dimethyl Ether is vaporized at 32 bar pressure and then mixed with the pressurized stream of Carbon Monoxide feed which contain 2% hydrogen as impurities at flowrate of 262 kmol/hr. This vapor mixture is pass through the reactor where

$$CH_3OCH_3 + CO \Leftrightarrow CH_3COOCH_3 \quad (2)$$

Reaction take place, where per pass conversion of Methyl Acetate is 89.22%. Reactor effluent is further cool to 320 K and flashed at 30 bar in flash drum which remove all unreacted gases from the stream and from that vapor stream small stream (13.1 kmol/hr) are purged to remove the Hydrogen. Other unreacted gases are again compressed at 32 bar and recycled to the pressurized Carbon Monoxide stream. Liquid outlet of flash drum are feed at 2nd tray of 17trays distillation tower(C3) which bottom product is Methyl Acetate. Top product of column C3 are compressed at 32 bar and recycled to the pressurized Carbon Monoxide stream. (*For more specification of all unit operation refer the main flowsheet or literature.*)

Problem identifies

Hence in selected literature is mainly focused on the alternative plant design and economy of plant, there are very less discussion about the thermodynamics. In Carbonylation route, due to the presence of hydrogen, we select Chao-Seader (which gives best result among other EOS) but still it gives some mismatch in phase equilibria prediction at flash drum (but it is still acceptable). DWSIM does not have vaporizer model directly so we use pump (for maintain pressure) and heater (to convert it into the vapor) instead of vaporizer.

Result

Feed and product stream data are given below

Object	Fresh Methanol Feed	Dimethyl Ether Produced	Fresh CO Feed	Methyl acetate Produced	Water	
Molar Flow	*500*	*247.624*	*262*	*246.908*	*252.37*	*kmol/h*
Methanol	0.99	0.001	0	0.001	0	mol/mol
Dimethyl ether	0	0.999	0	0	0	mol/mol
Water	0.01	0	0	0	1	mol/mol
Carbon Monoxide	0	0	0.98	0	0	mol/mol
Methyl acetate	0	0	0	0.999	0	mol/mol
Hydrogen	0	0	0.02	0	0	mol/mol

Conclusion

The selected flowsheet is simulated in DWSIM software by using their Unit operations and thermodynamics and result is match with literature in which, it was simulated by the commercial simulator; which prove the usefulness of open-source simulator DWSIM.

References

[1] R. B. Diemer and W. L. Luyben, "Design and Control of a Methyl Acetate Process Using Carbonylation of Dimethyl Ether," *Ind. Eng. Chem. Res.,* vol. 49, p. 12224–12241, 2010.