Production of Methyl Isobutyl Ketone from Acetone and Hydrogen

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Background:

Methyl Isobutyl Ketone (MIBK) can be produced by using low pressure one step gas phase process. Acetone and Hydrogen are used as a feed and nano-Pd/nano-ZnCr-O as a catalyst at about 1 atmospheric pressure. MIBK is generally used as a solvent for many industries. (1)

Process description:

Pure Acetone feed (S-01) and recycled acetone (S-26) is mixed in mixer (MIX-01). The mixed acetone feed (S-02) enters the Heat exchanger (HE -01), where it exchanges the Heat associated with the reactor effluent. The outlet stream (S-03) enters the heater (HEAT-01) for further heating and then to pressure reducing valve (VALV-01) before entering to the mixture (MIX- 02) and the conversion reactor (RC-01). Simultaneously Pure hydrogen feed (S-06) and recycled hydrogen (S-21) is mixed in mixer (MIX-03) .The mixed hydrogen feed (S-07) enters the heat exchanger (HE-03) and then heater (HEAT-02) for further heating and then to pressure reducing valve (VALV-02).Now , the mixed acetone feed stream (S-05) and mixed hydrogen feed (S-10) enters the mixture (MIX-02) and then the mixture (S-11) enters the Conversion reactor (RC-01).Where the conversion reaction takes place in the vapor phase with the average acetone conversion being specified as 70 %.The conversion depends upon the catalyst and various other parameters, so an average conversion of 70 % is taken. The reactor effluent contains unreacted acetone, unreacted hydrogen, MIBK and by-product as water. The reactor effluent (S-12) and (S-13) is mixed and stream (S-14) is obtained . (S-14) is recycled using (REC-01) which passes through (HE-01), (COMP-01), (HE-03), (HEAT -03). Stream(S-19) enters the compound separator (CS-01), where pure hydrogen (S-20) is obtained and recycled (REC-02) and mixed with pure hydrogen feed (S-06). The bottom product from (CS-01) i.e., stream (S-22) enters the Distillation column (DC-01) from which acetone obtained from the distillate is recycled (REC-03). The bottom product from (DC-01) enters the second distillation column (DC-02) from which mainly water (S-28) is obtained as distillate and pure MIBK is obtained as bottom product (S-29).

Flowsheet:

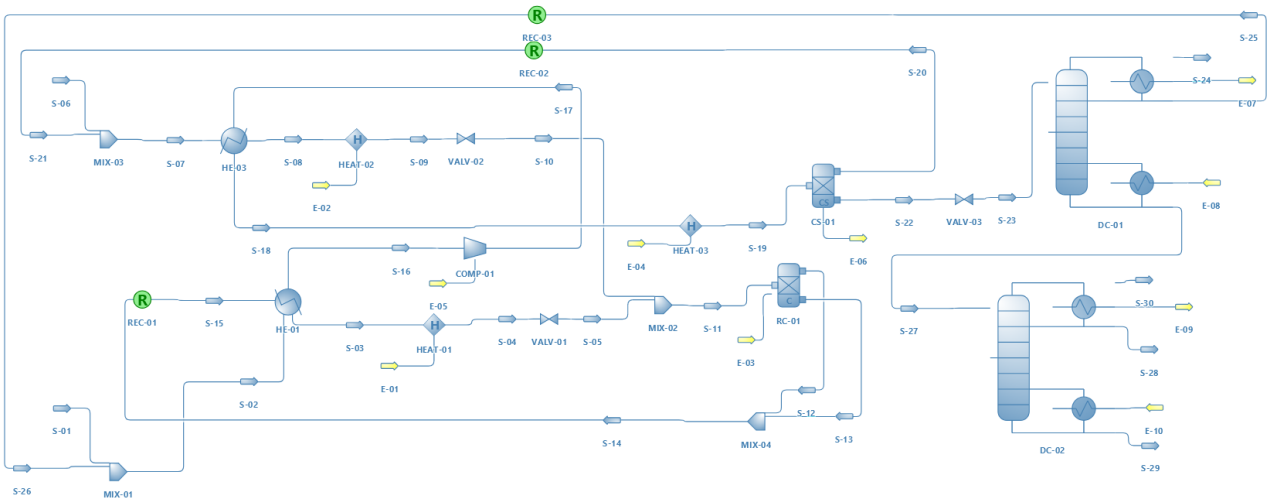


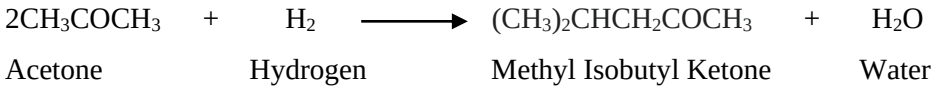
Figure 1:One step synthesis of MIBK

Results:

Master Property Table														
Object	**S-01**	**S-02**	**S-03**	**S-06**	**S-07**	**S-11**	**S-14**	**S-19**	**S-20**	**S-23**	**S-25**	**S-28**	**S-29**	
Temperature	343.15	338.912	623.15	298.15	302.761	622.709	788.354	308.15	308.15	308.15	338.994	377.066	385.544	**K**
Pressure	182385	141855	141855	597818	349572	121590	120590	101325	101325	101325	101325	101325	101325	**Pa**
Molar Flow	27.7778	60.3077	60.3077	14.0278	26.007	86.3147	72.4215	72.4215	12.1138	60.3077	35.1515	12.1562	13	**mol/s**
Volumetric Flow	0.00219969	0.00391242	2.20258	0.0581655	0.187268	3.67521	3.93629	0.385531	0.306291	0.00357447	0.0018625	0.000393228	0.00182738	**m3/s**
Molar Fraction (Mixture) / Hydrogen	0	0	0	1	1	0.301304	0.167268	0.167268	1	0	0	0	0	
Molar Fraction (Mixture) / Water	0	0.25775	0.25775	0	0	0.180089	0.406475	0.406475	0	0.488122	0.49995	0.858957	0.000682531	
Molar Fraction (Mixture) / Acetone	1	0.658207	0.658207	0	0	0.459886	0.164433	0.164433	0	0.197462	0.338613	0.00128365	2.76814E-23	
Molar Fraction (Mixture) / Methyl isobutyl ketone	0	0.0840431	0.0840431	0	0	0.0587205	0.261824	0.261824	0	0.314416	0.161437	0.139759	0.999317	

Conclusion and Recommendation:

- A flowsheet for continuous production of MIBK was built with a product purity of 99% with the open-source Simulation tool DWSIM- Version 6.4.8 Classic UI.
- Since kinetic data related to catalytic single step reaction is not available in the open-source literature, we have used a conversion reactor model in the flowsheet with average acetone conversion of 70%.
- NRTL model was used a thermodynamical model and only a ' Single-Step reaction ' with no intermediate reaction and no intermediate product takes place as follow.



References:

1. **Abdulrahman A. Al-Rabiah, Vagif Malik Akhmedov, Baku ,Abdulaziz A. Bagabas.** *LOW PRESSURE ONE-STEP GAS-PHASE PROCESS FOR PRODUCTION OF METHYL ISOBUTYL KETONE.* s.l. : US 2011 023783, 2011.