Effect of Flow Rate on Production of Butanal from Propylene, Carbon Monoxide and Hydrogen using Recycle Stream

Swetank Sahai

NIT Warangal

BACKGROUND AND DESCRIPTION

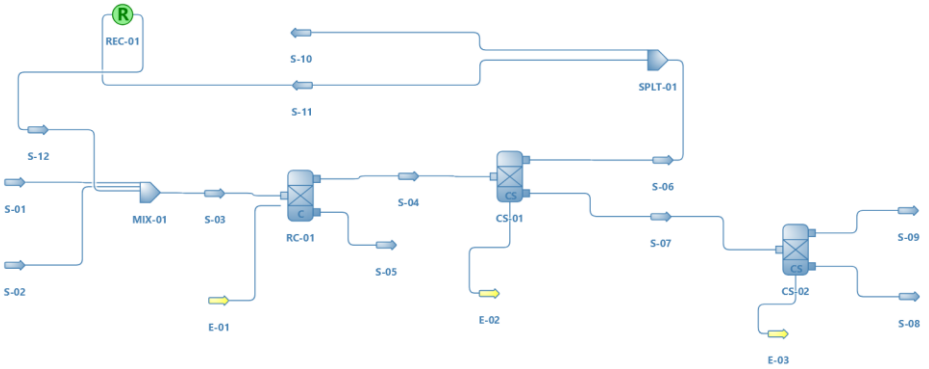
Hydroformylation of propylene to produce butanal is well known and practised widely. For economic reasons, the raw material used for such **industrial scale** processes has been propylene, which contains about 90-95 % **propylene**, with the majority of the balance being **propane**.

It is desirable that the unreacted propylene, carbon monoxide and hydrogen are **recycled and recovered**. It is also important to prevent excessive propane build up in the reaction system due to the recycle of the unreacted components. However, propane and propylene are difficult to separate and thus, in order to prevent propane accumulation, a purge stream is also required. This removal of propane however also involves the removal of some propylene resulting in some inefficiencies and economic debits in the process.

REACTION: $C_3H_6 + CO + H_2 \rightarrow C_4H_8O$

A feed Propylene containing traces of Propane(inert) is mixed with another stream of carbon monoxide and hydrogen along with a recycle stream and is then converted into butanal in the reactor. The total conversion with respect to Propylene is 0.9. Using compound separators, pure butanal as well as hydrogen/carbon monoxide streams as well as a recycle stream containing propylene and propane is obtained. However, to reduce the amount of inert, a purge is also established. Effect of inlet flow rate change on production is also observed.

FLOWSHEET



RESULTS

Material Stream

Master Property Table							
Object	S-01	S-02	S-03	S-04	S-05	S-06	
Mass Flow	2.10903	1.80156	4.05666	1.33399	2.72267	0.357226	kg/s
Molar Flow	50	120	173.399	46.477	38.0147	8.31227	mol/s
Molecular Weight (Mixture)	42.1805	15.013	23.3949	28.7021	71.6216	42.9758	kg/kmol
Molar Fraction (Mixture) / Propylene	0.95	0	0.284852	0.0993505	0.00846514	0.555506	
Molar Fraction (Mixture) / Propane	0.05	0	0.0231035	0.0794965	0.00819069	0.444494	
Molar Fraction (Mixture) / Carbon monoxide	0	0.5	0.346022	0.33449	3.85359E-06	0	
Molar Fraction (Mixture) / Butanal	0	0	0	0.152174	0.983336	0	
Molar Fraction (Mixture) / Hydrogen	0	0.5	0.346022	0.334489	4.75057E-06	0	

Master Property Table							
Object	S-07	S-08	S-09	S-10	S-11	S-12	
Mass Flow	0.976761	0.466786	0.509975	0.210763	0.146463	0.146463	kg/s
Molar Flow	38.1647	31.0921	7.0726	4.90424	3.40803	3.40803	mol/s
Molecular Weight (Mixture)	25.5933	15.013	72.1057	42.9758	42.9758	42.9758	kg/kmol
Molar Fraction (Mixture) / Propylene	0	0	0	0.555506	0.555506	0.555506	
Molar Fraction (Mixture) / Propane	0	0	0	0.444494	0.444494	0.444494	
Molar Fraction (Mixture) / Carbon monoxide	0.407341	0.500001	0	0	0	0	
Molar Fraction (Mixture) / Butanal	0.185318	0	1	0	0	0	
Molar Fraction (Mixture) / Hydrogen	0.407341	0.499999	0	0	0	0	

Reactor

PROPERTIES TABLE			
RC-01	Calculation Mode	Isothermic	
RC-01	Butanal production: Extent	90	%
RC-01	Propylene: Conversion	90	%
RC-01	Carbon monoxide: Conversion	74.0896	%
RC-01	Hydrogen: Conversion	74.0896	%

After Material Stream S-01 Flow Rate is increased from 50mol/s to 100mol/s,

Master Property Table				
Object	S-01	S-05	S-09	
Molar Flow	100	54.1216	9.97274	mol/s
Molar Fraction (Mixture) / Butanal	0	0.924348	1	

It is interesting to note that doubling the inlet flow rate does increase the butanal predominant streams, but the increase and yield is not sufficiently high to justify an increase in inlet flowrate.