Simulation of Production of Neopentyl Glycol

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Introduction

Neopentyl glycol is an organic compound which is used in as a raw material in the synthesis of polymer type chemical compounds such as polyesters, as additives for specific purpose polymers such as plasticizer in the manufacture of PVC and other chemical products such as lubricants and paints. The IUPAC name of neopentyl glycol is 2,2-dimethylpropane-1,3-diol and its structure is as shown in Fig 1.

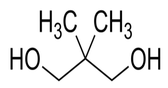


Figure 1: Structure of Neopentyl glycol

Not many processes for the manufacture of Neopentyl glycol exists. The main synthesis process involves aldol condensation of isobutyraldehyde and formaldehyde to produce hydroxipivaldehyde in presence of a basic catalyst. Hydroxypivaldehyde is further hydrogenated to produce neopentyl glycol. Heat of reaction for this aldol condensation reaction was estimated and found to be −60.4 kJ/mol, at 298 K. There are by products formed in this reaction sequence due to the Cannizzaro reaction but use of adequate operating temperature and pressure in the reactors along with catalysts can effectively reduce the yield of by products and increase selectivity of the desired product. Furthermore, appropriate separation processes such as distillation and flash separation can be employed to get a high purity of the desired product.

Objective

The main objective of this project is to intoduce the production of neopentyl glycol through ASPEN software. And to simulate the whole production process.

Manufacturing process

The entire process of manufacture of neopentyl glycol can be divided into three sections:

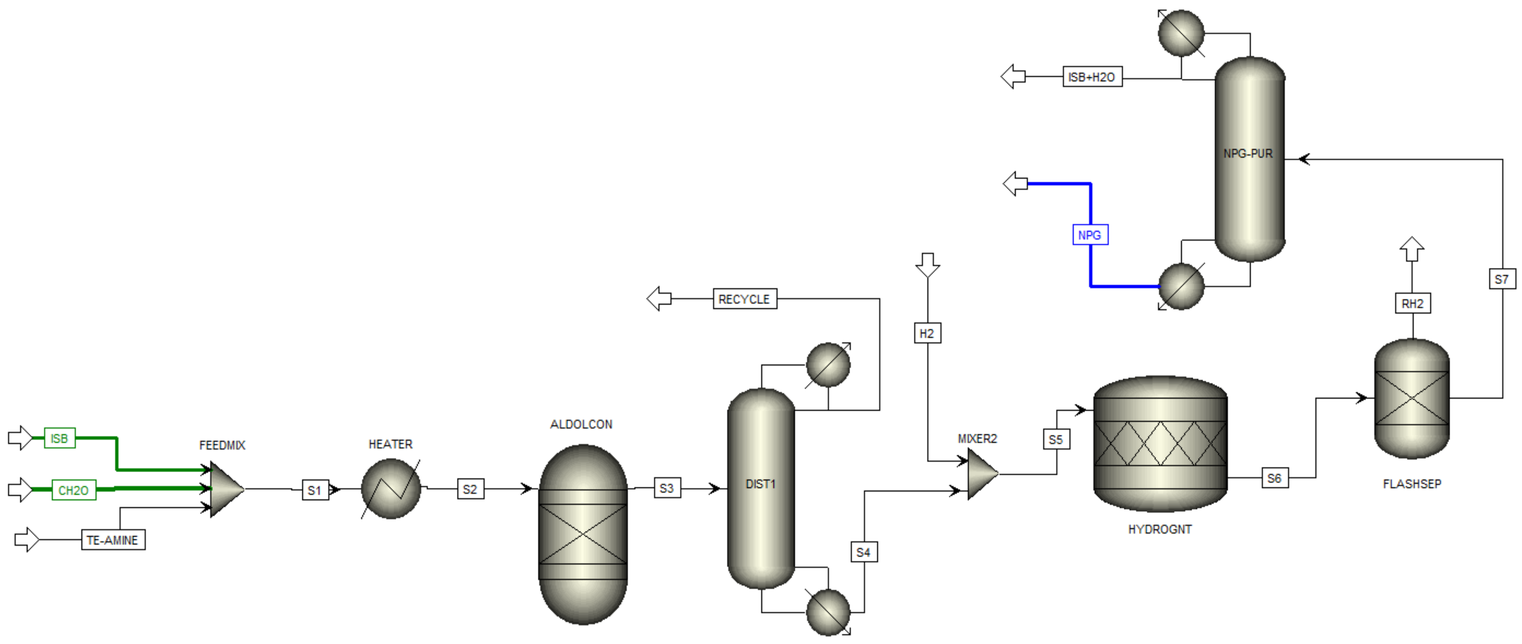
- Aldol condensation and separation of products.
- Hydrogenation
- Purification

The first step of the manufacturing process involves aldol condensation of isobutyraldehyde and formaldehyde in presence of a base. It is mentioned that weak basic anion exchange resins, with tertiary amines as active groups are best suited for catalysing the aldol condensation reaction. In this project work, triethyl amine has been considered as the catalyst. The resultant aldol product contains unreacted isobutyraldehyde which can be separated by distillation. The bottom product contains hydroxypivaldehyde in a relatively larger fraction and is forwarded for hydrogenation reaction which is the next step.

Hydrogenation of hydroxypivaldehyde has been studied in various scientific research works and noteworthy is the work of Mikio who studied the hydrogenation of hydroxypivaldehyde using bimetallic Ru–Pd on carbon catalyst at 373K and elevated hydrogen pressure. In the considered Aspen model, hydrogenation was carried out in a stoichiometric reactor with known conversion of hydroxypivaldehyde. The unreacted hydrogen is separated from the products of hydrogenation using a vapor liquid separator. This hydrogen can be vented out to maintain fresh hydrogen feed in the catalyst bed of the reactor or it can be reintroduced along with the fresh feed into the reactor.

The final step of manufacture involves purification of the hydrogenation products through a distillation column for getting a higher purity of neopentyl glycol in the bottom product. The midpoint of the column is fed product from the hydrogenation and a 10 percent sodium hydroxide solution which provides caustic to saponify the esters present in the hydrogenated product and to liberate triethylamine from its carboxylic acid salts. This step is omitted in the model considered as the Cannizzaro side reaction during aldol condensation and the esterification side reaction during hydrogenation of hydroxypivaldehyde are assumed to have very low yields and are hence neglected. Top product of the column contains methanol, isobutanol, triethylamine, and water.

Design and Process Flow Diagram



Results and Discussion

	Units	ISB	TE-AMINE	CH2O	NPG
From					NPG-PUR
To		FEEDMIX	FEEDMIX	FEEDMIX	
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN
Maximum Relative Error					
Cost Flow	$/hr				
MIXED Substream					
Phase		Liquid Phase	Liquid Phase		Liquid Phase
Temperature	C	25	25	25	206,014
Pressure	bar	1,01325	1,01325	1,01325	1
Molar Vapor Fraction		0	0	0,450545	0
Molar Liquid Fraction		1	1	0,549455	1
Molar Solid Fraction		0	0	0	0
Mass Vapor Fraction		0	0	0,575133	0
Mass Liquid Fraction		1	1	0,424867	1
Mass Solid Fraction		0	0	0	0
Molar Enthalpy	cal/mol	-59226,3	-31264,2	-49940,6	-116746
Mass Enthalpy	cal/gm	-821,368	-308,959	-2143,36	-1124,38
Molar Entropy	cal/mol-K	-100,913	-191,454	-23,5676	-147,407
Mass Entropy	cal/gm-K	-1,3995	-1,89199	-1,01148	-1,41967
Molar Density	mol/cc	0,0108962	0,0073477	9,19787e-05	0,00827607
Mass Density	gm/cc	0,785688	0,743528	0,00214311	0,859315
Enthalpy Flow	cal/sec	-16451,7	-868,449	-13872,4	-13621,5
Average MW		72,1069	101,192	23,3001	103,831
Mole Flows	**kmol/hr**	**1**	**0,1**	**1**	**0,420035**
Mole Fractions					
Mass Flows	**kg/hr**	**72,1069**	**10,1192**	**23,3001**	**43,6128**
Mass Fractions					
ISOBU-01		1	0	0	0,000952982
FORMA-01		0	0	0,567017	1,39224e-08
TRIET-01		0	1	0	0,000418588
METHA-01		0	0	0	0
ISOBU-02		0	0	0	0
NEOPE-01		0	0	0	0,900415
WATER		0	0	0,432983	0,00014394
HYDRO-01		0	0	0	0
HPA		0	0	0	0,0980694
Volume Flow	l/min	1,52959	0,226828	181,201	0,845884

It can be observed that the product stream NPG has appreciable purity for neopentyl glycol, 89.76% on mole basis and 90.04% on mass basis. The streams RECYCLE and ISB+H2O consists of considerable amount of isobutyraldehyde and water which can be recycled to the feed for process economy.

Total molar flow of feed is 2.1 kmol/hr compared to the total molar flow of main product Neopentyl glycol 0.425 kmol/hr. Most of the molar flow is lost at the top products (RECYCLE) in the distillation step (DIST1) after adol condensation. Hence, the top product should be recycled for compensating the loss of material. 46.07% extracted hydrogen relative to the fresh hydrogen was recovered in the flash separator, which can be recycled back and mixed with the fresh hydrogen feed.

Conclusion

The model simulated yields a sufficiently pure neopentyl glycol: 89.76% on mole basis and 90.04% on mass basis. The product flow rate is low as compared to the feed flow rate but the loss of material is identified to happen at the distillation stage and the stream RECYCLE can be recycled to mix with the initial feed for reducing loss of material.

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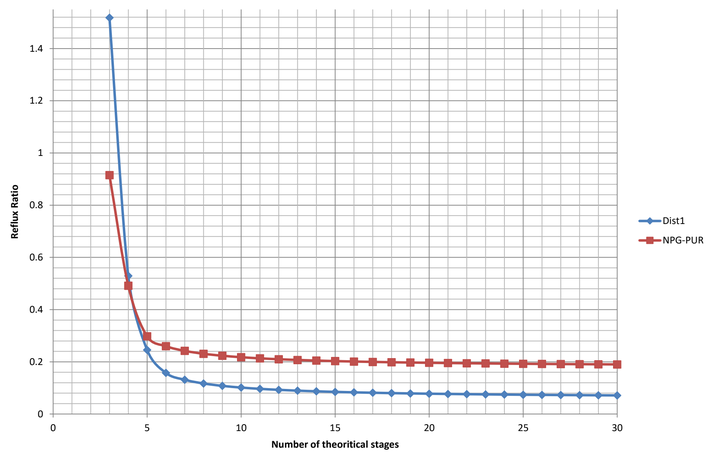
Analysis Dist columns



The distillation columns for separating the aldol condensation products and the hydrogenation products have been analysed for reflux ratio vs number of stages to understand the optimisation of number of stages and the reflux ratio. Increasing number of stages involves initial capital investment whereas it decreases the reflux ratio meaning increasing the flow of products meaning more revenue from products for the process. A compromise has to be made between the two parameters which is based on economic consideration. The top product of final purification by distillation (NPG-PUR) has a high content of isobutyraldehyde and water which can be recycled back to the feed as well. Furthermore, the unreacted hydrogen extracted using a flash separator can be recycled to mix with the fresh hydrogen feed as well

Future work

The recycle of top products of distillation of the aldol condensation products which contains significant mass flow of unreacted materials was attempted as shown in Figure II in Appendix. Error in the mass balance occurred during simulation which can be investigated further and rectified for a more efficient model.

Cannizzaro reactions during aldol condensation has been neglected in this model which yields salts. Similarly, esterification reaction occuring during hydrogenation of hydroxypivaldehyde due to self condensation is also neglected in this model. Such side reactions can be considered for further investigation on their effect on the process. Subsequently, saponification, salt removal and drying units can be added to the purification process of neopentyl glycol.

Economic analysis on distillation columns based on number of stages, height of the column and reflux ratio optimisation can be carried out.