Simulation of Production of Neopentyl Glycol

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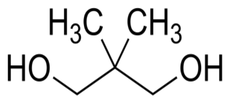
Introduction

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 the figure below.



- 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.
- Furthermore, appropriate separation processes such as distillation and flash separation can be employed to get a high purity of the desired product.

Objective

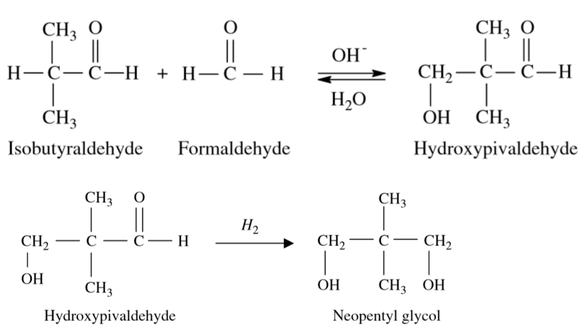
- Modelling and simulation of manufacture of Neopentyl glycol.
- Identifying and optimizing processes giving low yield of desired product
- Literature survey to compare the model with existing processes
- Employing recycle streams wherever necessary
- Suggesting improvements in the model

Manufacturing process

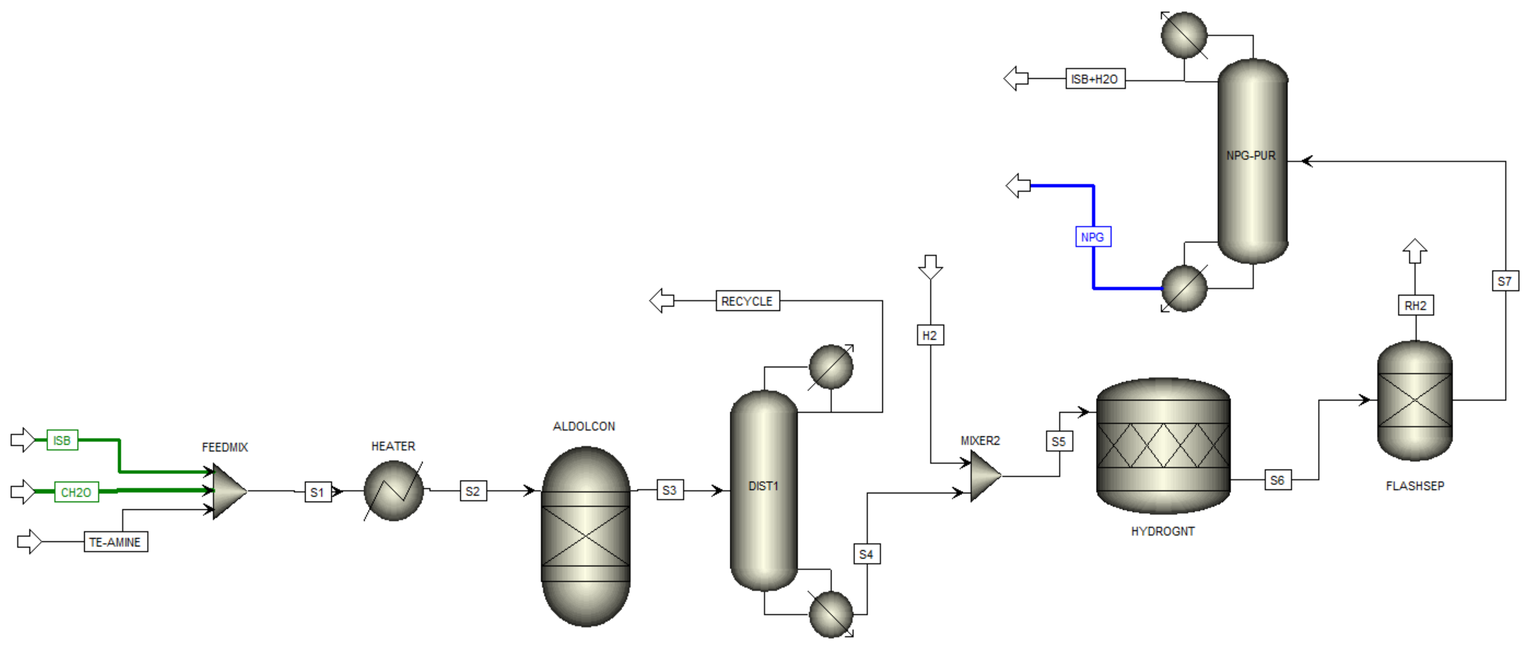
The entire process of manufacture of neopentyl glycol can be divided into three sections:

- 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 from hydroxypivaldehyde.
- Hydrogenation of hydroxypivaldehyde has been studied in various scientific research works and the hydrogenation of hydroxypivaldehyde using bimetallic Ru–Pd on carbon catalyst at 373K and elevated hydrogen pressure is a noteworthy work.
- 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.
- 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. 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

- 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 has 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.
- Top product of DIST1 to be recycled for compensating the loss of material.
- 46.07% extracted hydrogen relative to the fresh hydrogen at FLASHSEP.

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 DIST1 and the top product stream can be recycled to mix with the initial feed for reducing loss of material.

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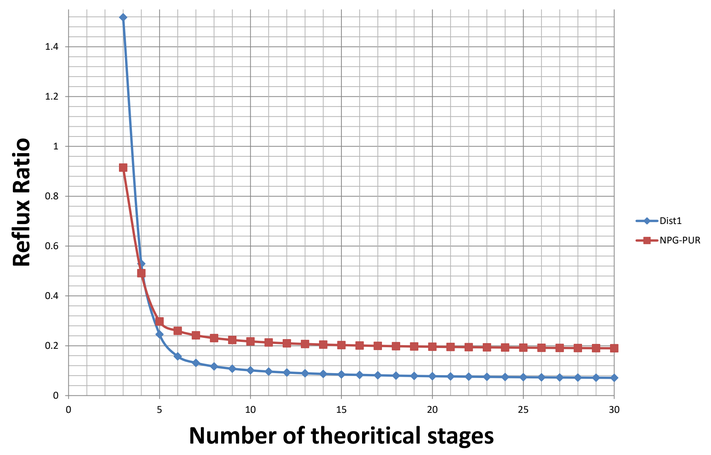
Analysis of distillation



- 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.
- Increasing reflux ratio also increases heat duty of the reboiler of the distillation column.

Future work

- The recycle of top products of distillation of the aldol condensation products which contains significant mass flow of un-reacted 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 occurring 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.